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Triggers for Chemical Product Design: A Systematic Literature Review

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ABSTRACT

The product design project is a complex problem because objectives and constraints must be considered simultaneously, the sustainability context is highly relevant and specific, decision-making involves not only customer needs but also of other stakeholders, especially the organization in which the design project takes place. This work presents a systematic literature review of design methodologies for chemical products to identify how that problem has been addressed and which are the future challenges to be met. The review involved the analysis of 262 research papers and 336 patents, classified according to the chemical product type, the design phase studied, and whether they consider association with a business context. The study highlights the need for holistic product design methodologies applicable from the early design stages, covering the assessment of customer needs and the requirements of other stakeholders, as well as the business context where the design process is carried out.

Keywords

Chemical product design, formulated product, business, enterprise strategy, product design methodology, company, consumer products, cosmetics, patents.

INTRODUCTION

The design of formulated consumer products is a major challenge in many industrial sectors from both a technical and a business point of view ^{1,2}. In that type of chemical products, properties are conferred by a synergistic action of ingredients, composition, and production process. Thus, the solution space contains multiple solutions ^{3,4} considering the combinations of the three variables mentioned previously. That large solution space should be reduced to satisfy not only the expectations of consumers but also the requirements of other stakeholders, highlighting those of the company where the product is designed ⁵. In this sense, the product design process must be in line with the business strategy and operations of the company where it is developed.

The design process of chemical products comprises (1) the study of consumer needs and their translation into technical requirements, (2) the conceptualization of the product, the selection of raw materials and suppliers, and (3) the establishment of environmental objectives, marketing characteristics, sales, and distribution goals ⁶. It is a multi-objective and multi-stakeholder process, which constitutes a major problem for enterprises because they must manage information and knowledge related to the design variables throughout the whole product design and development project ⁷.

Product design is an activity that normally occurs within a company, which can greatly limit or foster the decisions made by the design team. Moreover, organizations or enterprises that incorporate design as part of their activities have shown a positive effect on their business development and evolution ⁸. Despite the above, to the best of our knowledge the business context has not been fully included in most of the chemical product design methodologies that have been proposed and published. In general, most methodologies found in the literature have a weak connection to consumer awareness and decisions in a business context ⁹.

Some approaches have partially incorporated it. For example, Ng¹⁰ highlighted the relation between business and chemical product design and proposed a framework for hierarchical decision-making within a company. Nevertheless, that approach considered only large-sized enterprises, without the analysis of user needs which is essential for consumer products, and the decision-making strategy was based only on a financial return function. For their part, Fung et al. ¹¹ proposed a product design model comprising six sub-models: process, property, quality, cost, pricing, and economic model. They pointed out the importance of some business elements, such as corporate strategy, marketing, government policies, and regulations. However, these variables were not implemented in the case study developed to illustrate the design process. Smith & Lerapeprou ¹² identified practical issues that inhibit a connection between business decisions and chemical product design decisions. Among these issues, they found a lack of (1) historical data for the interpretation of market needs and

preferences, (2) common variables and restrictions used to describe sustainability features, and (3) restrictions imposed by new regulations. Finally, Heintz et al ¹ presented a methodology for product design where the restrictions and rules posed by the strategic and tactical dimensions of the company are brought together in the same common system language to set operational restrictions, allowing the designer to introduce a common framework for sharing information across the enterprise.

Given the above, this work presents a comprehensive bibliometric study of the existing chemical product design methodologies, emphasizing the design phases defined, the product types addressed, and the aspects related to the business context which is considered. The main objective is to identify the aspects still not considered up to now and the research challenges of proposing a novel chemical product design methodology within a company context. Some key aspects of this methodology can also be incorporated in chemical engineers training, which may require developing new competences, namely those related to customer needs comprehension, business and interdisciplinary skills, to respond to the chemical product design problems. The review is structured as follows: Section 2 presents the background explaining different product design methodologies and the business context considered in this assessment. Section 3 explains in detail the methodology applied to develop the bibliographic study. Section 4 presents the results of the analysis by classifying the existing contributions into product type, design phase, and whether or not they present a business approach. Finally, Section 5 identifies the main contributions and future challenges in the research of chemical product design within companies.

BACKGROUND IN CHEMICAL PRODUCT DESIGN AND BUSINESS MODELS

Chemical product design

In the chemical industry, the design process is focused on obtaining either products, processes, equipment, or production plants with specific characteristics. Chemical product design aims to define a set of molecules, formulations, or devices to fulfill a set of requirements to satisfy customer needs in a sustainable way considering external and internal restrictions ¹³. It also seeks to define how to produce these products. Thus, in the current state of the art, chemical process design is a part of chemical product design ¹⁴, the objective of which is to define a set of operations and process flow diagrams allowing the engineer to design, construct, start-up, and operate a process plant where raw materials are transformed into products that meet specifications in a sustainable way, considering external and internal restrictions ¹³. During plant design, the design team produces a set of diagrams, drawings, specifications, lists, and data sheets to perform the procurement, construction,

commissioning, and operation of a process plant in a sustainable way¹³. The last two are well-known design tasks that are highly studied by the academic community and applied daily by chemical engineers. In contrast to them, chemical product design is a relatively new research field. Even though there are several computer-aided methods and tools suitable for chemical-based product design¹⁵, most of these have not yet been adapted to solve practical industrial problems¹⁶. Moreover, given the wide diversity of products and their differences, one main theoretical question of this study is to identify whether there is a generic chemical design methodology suitable for all types of chemical products and, if this does not exist, then to determine the applicability and limitations of the existing ones.

Cussler and Moggridge¹⁷ established four types of chemical products: commodities, devices, molecules, and micro-structures. Commodities (e.g. sulfuric acid, methanol, ethylene, etc.), are generally described in terms of purity and market price; their design process seeks to improve process conditions, the conversion and selectivity of chemical reactions, environmental factors, or energy integration¹⁸. Devices (e.g. ozone generator, domestic water filter, mist humidifier, continuous positive airway pressure (CPAP) system, etc.) are miniaturized chemical processes transferred to the end-user with operating and safety conditions defined by the application; their design is based on the development of intellectual property and follows principles of chemical processes and chemical reaction engineering¹⁹. Molecules (e.g. ibuprofen, penicillin, tadalafil, styrene) are pure chemical compounds usually associated with specific chemical or biological functionalities. Their design process is related to the opportunity of their discovery; techniques such as the group contribution (GC) and Quantity-Structure-Property-Relationship (QSPR) methods²⁰⁻²² are used to model and optimize them. Micro-structured chemicals (e.g., adhesives, coatings, films, cosmetics, etc.) are characterized by their end-use properties, which must respond directly to the consumer's needs. These properties are yielded by the synergy between their ingredients and the manufacturing process, which together create a formulation with a microstructure and specific characteristics and behavior.

Some other authors propose other classification systems, as shown in

Table 1, based on criteria such as product complexity, chemical nature, and application, among others. All the classification systems presented are complementary, and other classifications are possible. In this article, the classification system proposed by Cussler and Moggridge¹⁷ is highlighted because it connects the product with the key design stage(s) and the key design variable(s). In addition, special attention is given to the micro-structured products because most end products belong to this product type and their design involves the challenge of simultaneously considering ingredients and the manufacturing process. For instance, in the work presented by Taifouris et al²³ this kind of product is addressed as part of the largest set of formulated products; elsewhere they are listed in the classification of chemical specialties²⁴.

Table 1. Chemical product types in different classification systems

	Classification criteria of chemical products				
	Chemical nature/micro-structure			Product complexity	Application
Categories of chemical products	<ul style="list-style-type: none"> • Commodities • Molecules • Devices • Structures 	<ul style="list-style-type: none"> • Molecules and blends • Devices and functional products • Formulated products 	<ul style="list-style-type: none"> • Devices • Molecules • Structures 	<ul style="list-style-type: none"> • Basic/functional chemicals • Structured products • Configured consumer products 	<ul style="list-style-type: none"> • Coatings and sensors • Process fluids • Fertilizers and pesticides • Food • Healthcare • Skin protection • Dyes and pigments • Fragrances • Special separations • Energy provider • Reaction promotion • Functional device
Reference	*17	25	26	12	16

*Note: For the analysis of the publications, this classification of chemical products is applied.

Independently of the product classification system, clear and radical differences can be observed in different chemical product categories, making difficult to propose a universal design methodology for chemical products. Thus, different methodologies have been adapted to each specific product type, selecting the most appropriate tools and solution strategies according to the design problem. This review is focused on formulated chemical products, understanding that the design of formulated products is highly dependent on the choice of ingredients and their manufacturing process. Additionally, special attention is given to consumer products, as in the case of cosmetic ones.

Cussler and Moggridge ¹⁷ proposed at least four phases for the design of formulated chemical products:

- Identification of needs: understanding the needs of the client.
- Generation of ideas: generating product alternatives that satisfy those needs.
- Idea selection: selecting the most prominent alternative.
- Process design: carrying out its production.

The business model in methodologies for chemical product design

Recently, companies in the chemical sector have been moving from commodity to specialty chemicals or even more differentiated products, such as consumer-driven products ²⁷. This is the result of new corporate strategies ¹⁷ that search for markets with high added value, responding to new demands such as sustainable production and development of highly specialized products ¹⁰. For these products, design is based on decisions made by multidisciplinary teams, not always directly related to the design activity ²⁸, which interact within a corporate context. As part of the activities of a company, product design projects are framed in the operation of business departments (such as marketing, sales, research and development, production) or a team that makes up part of a larger organization. Businesses are characterized by having operational (short-term) and tactical (medium-term) objectives, which are aligned with the business strategy of the organization (long-term goals that mark the organization's expected future, connected in turn with the company mission, meaning the company's *raison d'être*, and vision, meaning the organization's future) ²⁹.

Decisions made within a design project, which is developed over a period of six months to two years, are tactical and operational. They involve more than one business department, and they are made on the one hand to satisfy the needs of customers and on the other hand to respond to other stakeholders, involving the same company in which the project is carried out. Due to the above

factors, the product design process must be aligned with corporate strategies that transfer value and differentiation to the products ³⁰.

The decision-making during a design project, as well as the flow of information inside the company, can be represented by a business model. Business models are useful for establishing or visualizing how companies organize themselves to operate for value creation and delivery ³¹, an activity that is strongly driven by innovation and design. Every company uses business models explicitly or implicitly, and in them it is possible to evidence key design aspects such as customers' needs and clients' financial potential, as well as the relationships with other stakeholders influencing the decision-making process, among others ^{31,32}. For instance, in the cosmetic sector some new trends, such as the use of multifunctional products and the interest in organic products, demand an accelerated product design, development, and launch ³³. Assuming that a cosmetic company's tactical objective is to respond to such trends with new products, the design process within that company must consider the possibilities and constraints of developing new products (particularly in terms of time). In other words, the company is the context where the design activity is developed, and the business model represents the information and interrelations within the companies. In the particular case of cosmetic products, companies face a highly competitive market environment that by the end of the year 2018 reached approximately 200 billion, with a compound annual growth rate close to 5.5% and a positive growth behavior over the last decade ³³. Thus, the design processes applied by companies must meet market demands in terms of trends, value promise, development time, and product costs ³⁴, and offer new propositions at the same time.

One of the interests of this study is to identify the extent to which the chemical product design methodologies have addressed the business context of an organization. Particular attention is given to those methodologies in which information flows related to business strategies, such as the value proposition, are evidenced.

LITERATURE REVIEW

A bibliometric analysis was carried out to identify the extent to which chemical product design has been studied in a business context. The methodology used for developing the bibliometric analysis is presented in Figure 1. It comprises three phases: research equation definition, first classification, and deep analysis. The methodology was applied for two types of documents: scientific publications in chemical product design and patents related to cosmetic products.

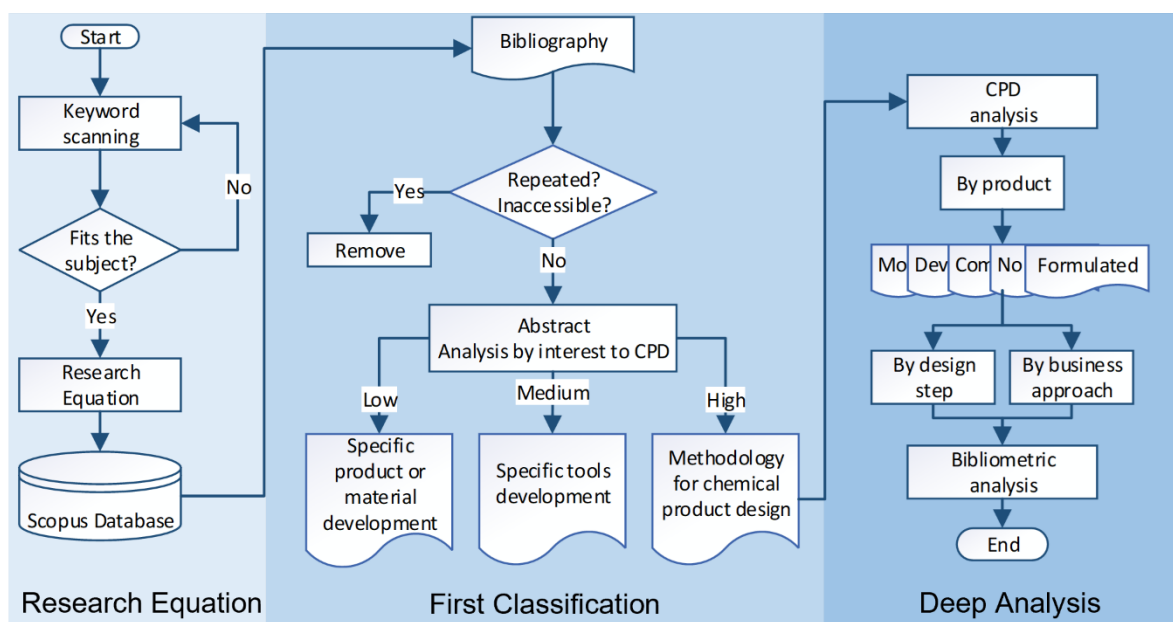


Figure 1. Methodology for bibliometric analysis

For the analysis of scientific publications, in the phase of *research equation definition*, a scanning of keywords was done using the Scopus search engine. The keywords and their combinations with more results were used to compose the research question. The search was limited to journal articles, conference papers, and reviews. The search period was restricted to the period from 1995 to August 2020. The search equation comprises the keywords “chemical products design” and “methodologies” or similar in all search fields, as presented in Equation 1. The Boolean operator AND was used to force the result to include all the equation parts, the operator OR was used to include at least one option within the brackets, and wild cards like * to avoid issues with plurals or derived words.

Equation 1. Bibliometric search equation

$$\left(\begin{array}{c} \text{"chemi* product* develop*"} \\ \text{OR} \\ \text{"chemi* product* design"} \end{array} \right) \text{AND} \left(\begin{array}{c} \text{method*} \\ \text{OR} \\ \text{approach} \\ \text{OR} \\ \text{decision making} \end{array} \right)$$

For the second phase, the *first classification*, a screening was carried out. Those documents which were repeated or inaccessible were eliminated from the list. Then, the abstracts were read and sorted according to their relation to the topic studied. Three categories were established for this classification: low, for those documents whose content is not of interest for this study; medium, for papers that are related to product design in the chemical industry but not to design methodologies; and high for papers that specifically deal with the development of chemical product design methodologies.

For the phase of *deep analysis*, three sub-classifications were defined according to three criteria: type of chemical product (commodities, molecules, devices, formulated), design phases considered in the methodology (needs analysis, needs translation, alternatives proposition, selection, and process design), and if there is a business approach (it was identified if elements of the business strategy or activities conducted by a business context were considered within the proposed design methodology).

In our final bibliometric phase, an analysis of patents related to the subject was carried out. In this case the search was focused only on one application sector: cosmetic products, due to our interest in methodologies developed for cosmetic products because they are an example of formulated consumer products. Their design is a challenging research subject because it must be designed based on customer needs, which are frequently subjective and difficult to translate. Additionally, in this type of product the micro-structure partially defines product characteristics, and this requires a

simultaneous design of the product and the process. A more specific search equation was implemented. Equation 2 shows the search terms applied to the cosmetic patents. For this search the online tool PATENTSCOPE by WIPO (World Intellectual Property Organization) was used.

Equation 2 Patent search equation

*(Cosmetic*AND design AND method*)*

In this search, 336 patents were found to meet the criteria. Then, an analysis by title, abstract, and proposal of the invention was performed.

RESULTS

SCIENTIFIC PUBLICATIONS

For the scientific publications (journal articles), 658 documents were selected after the redundant and inaccessible documents were screened out. Subsequently, these documents were classified by their relevance to this study, as high, medium, or low. A total of 257 documents were classified as highly relevant, as shown in Figure 2.

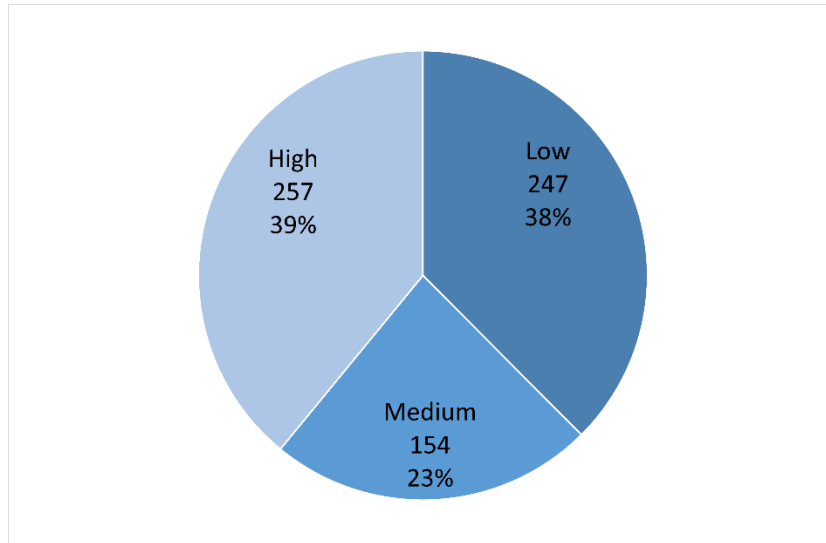


Figure 2. Results of the first classification of documents in scientific journals according to relevance to the subject

Only the high-relevance documents (257) were analyzed further.

Table 2 presents the results of this classification only for the publications related to the product type Formulated Products (which comprises 126 publications).

Table 2. Publication summary regarding formulated chemical products.

Ref.	Product type				Design phase					Business approach		Sector
	Com	Mol	Dev	For	Nea	Tra	Alt	Sel	Pro	Stru	Stra	
35				X	X	X	X	X				Cos.
36				X			X					Pha.
37				X	X			X		X		Un.
38				X	X		X	X				Pha.
39				X	X	X	X	X		X		Un.
40		X		X	X		X	X	X	X	X	Un.
41	X			X			X					Pol.
42				X			X	X				Cos.
43	X			X			X					Pol.
44				X				X		X		Cos.
10				X	X		X	X	X			Un.
45				X	X		X	X		X		Un.
46				X	X		X					Pha.
47				X	X		X					Cos.
48				X			X		X			Un.
49				X		X						Food.
50				X			X	X	X			Un.
51				X	X		X	X				Food.
52				X				X	X	X		Pha.
53				X	X		X	X				Food.
54				X			X					Pha.
55				X	X		X	X	X	X		Food.
56				X			X		X			Cos.
57				X	X		X	X		X		Cos.
58		X		X			X	X	X			Ink.
59				X	X	X				X		Cos.
60				X			X	X				Pha.
61				X	X		X	X				Hom.
62				X			X	X				Hom.
63				X			X		X			Ink.
64				X		X				X		Pha.
65				X			X	X				Food.
66				X	X		X	X		X		Cos.
67				X	X	X	X					Food.
68				X			X		X			Un.
69				X			X	X				Cos.
70				X			X	X				Ink.
71				X			X	X				Cos.
72		X		X				X		X		Ink.
73				X					X			Un.
74				X			X	X				Cos.
75	X			X			X	X	X			Ink.
75				X				X				Cos.
76				X			X	X				Ink.
77				X			X					Ink.
78				X			X					Ink.

Ref.	Product type				Design phase					Business approach		Sector
	Com	Mol	Dev	For	Nee	Tra	Alt	Sel	Pro	Stru	Stra	
79				X	X	X		X	X			Hom.
80				X				X		X		Un.
4				X	X		X	X	X			Hom.
81				X			X					Ink.
1				X	X		X	X		X	X	Ink.
82				X			X	X				Ink.
83				X			X	X				Ink.
83				X	X	X	X					Cos.
84		X		X	X		X	X				Ink.
85		X		X	X		X	X				Ink.
86				X			X	X				Cos.
87				X			X	X				Pha.
88				X			X	X				Ink.
89				X	X		X	X		X		Cos.
90	X			X	X	X						Ink.
91				X			X	X				Pol.
92		X	X	X	X		X	X				Cos.
93				X	X		X	X				Ink.
94	X			X			X	X		X		Ink.
95				X			X	X				Ink.
18	X			X	X		X	X				Ink.
96				X			X	X	X			Hom.
97				X	X		X	X		X	X	Pol.
98				X	X	X	X	X				Pol.
99				X	X	X	X	X		X		Food.
100				X	X			X				Ink.
101				X			X	X				Ink.
102				X			X	X				Ink.
103		X		X			X	X				Ink.
104				X			X	X				Ink.
105		X		X			X	X	X			Food.
106				X			X	X				Ink.
11		X	X	X	X	X	X	X	X	X	X	Ink.
107				X	X		X	X		X		Un.
108				X	X	X	X	X				Ink.
109				X			X	X				Ink.
110				X			X	X				Ink.
111				X				X				Pol.
112				X			X	X				Ink.
113				X			X	X				Ink.
114		X		X	X		X	X				Un.
115				X	X		X	X				Hom.
116				X			X	X				Pol.
117				X				X				Ink.
118				X				X				Hom.
119	X	X		X			X	X				Ink.
120				X	X	X	X	X				Cos.
121				X	X		X	X				Ink.
122				X	X			X				Food.

Ref.	Product type				Design phase					Business approach		Sector
	Com	Mol	Dev	For	Nee	Tra	Alt	Sel	Pro	Stru	Stra	
123				X	X		X	X			X	Food.
124				X			X	X				Cos.
125		X		X	X		X	X				Ink.
126				X	X		X	X		X	X	Pol.
26				X	X	X	X	X	X			Cos.
127				X	X		X	X				Cos.
128				X			X	X				Ink.
129				X	X	X	X					Cos.
130				X	X		X	X	X	X	X	Ink.
131				X				X				Ink.
132				X			X	X				Un.
133				X			X	X				Ink.
134				X			X	X				Ink.
135				X			X	X		X		Hom.
136				X			X	X				Pol.
137				X	X	X	X	X	X			Food.
138				X			X	X				Pol.
139				X			X	X				Ink.
140				X	X		X	X		X		Cos.
141				X			X	X				Ink.
142				X			X	X				Un.
143		X		X			X	X	X			Ink.
144		X		X			X	X		X	X	Pha.
145		X		X			X	X				Ink.
146		X		X			X	X	X	X	X	Ink.
147				X			X	X				Hom.
148				X				X				Cos.
149				X				X				Ink.
150				X			X	X				Ink.
151				X				X				Cos.
152				X			X	X		X		Ink.

(Product types: Com. = commodities, Mol. = molecules, Dev. = devices, For. = formulated. Design phase: Nee. = need analysis, Tra. = needs translation, Alt. = alternatives proposition, Sel. = selection, Pro. = process design. Business approach: Stru. = business unit structure, Stra. = business strategy. Application: Cos. = cosmetics, Pha. = pharmaceuticals, Pol. = polymers and materials, Food. = food industry, Hom. = homecare, Ink. = solvents-fluids-paints-inks, Un. = unspecified)

Figure 3 shows over time the upward trend of the scientific journal publications in the category of high relevance. Around 50% of the documents were produced in the last six years, which shows there is recent and increasing interest in researching chemical product design methodologies, notably those articles applicable to integrated and multiscale product design as presented in ^{137,142,143,153}.

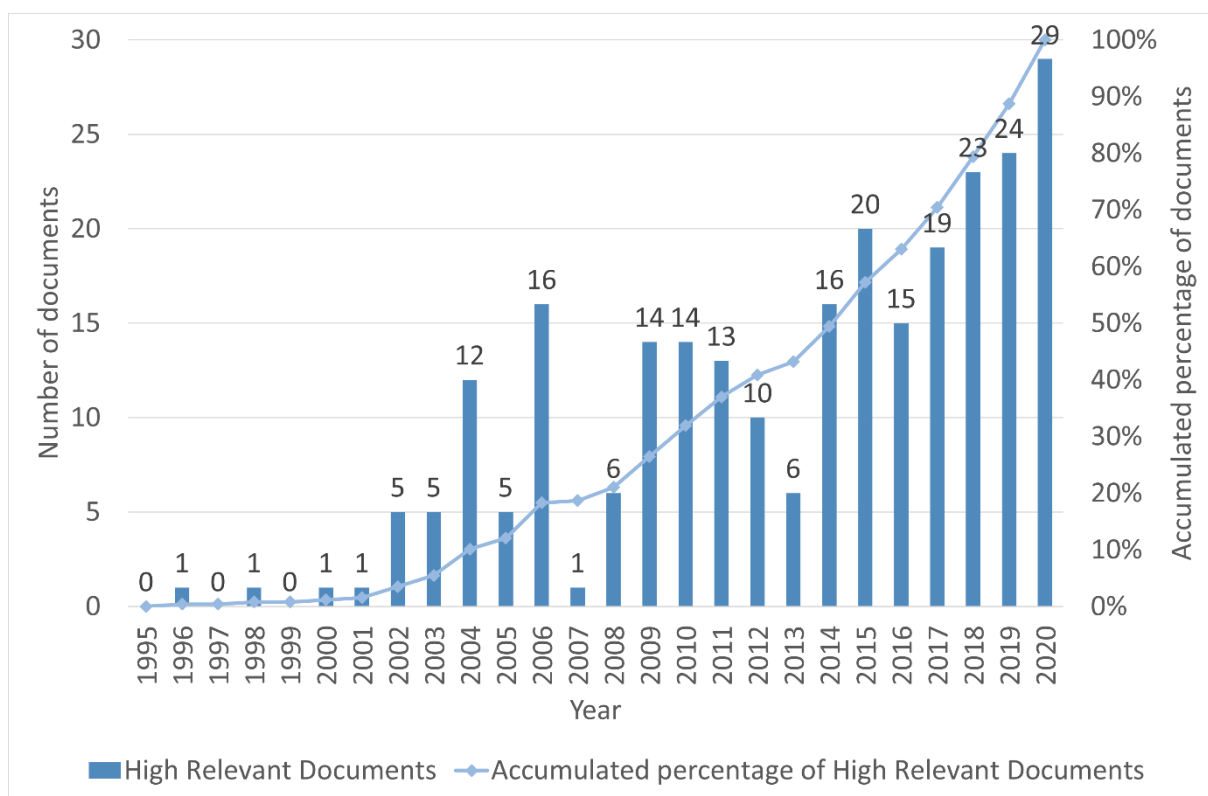


Figure 3. Evolution of publications in scientific journals concerning chemical product design methods for highly relevant documents

Product types

Of the 257 publications in the high-relevance category, 206 can be analyzed under our analysis methodology. The remaining 51 papers are reviews and state of the art related to the topic documents, as well as articles from industrial and academic perspectives. Figure 4 shows the results of the classification according to the chemical product type (commodities, molecules, devices, formulated). It was found that 183 documents (89%) focus on a single product type, remarkably formulated products, and molecules, with 104 and 61 documents, respectively. Twenty publications (10%) correspond to two product types, and three to three product types (1%). In the case of formulated products, many of the methodologies consider an interdisciplinary approach, where aspects such as product properties, marketing, costs, management, and process design are combined or at least mentioned when presenting a design methodology^{137,142,143,153}. Formulated products are frequently found in the consumer market, thus the inclusion of multiple variables and the application of interdisciplinary knowledge is necessary for their design^{59,122,123}.

Regarding the articles that only mention the product type Molecules, the extensive use of tools for computer-aided molecular design (CAMD) is evident. These tools aim to define molecules or their mixtures with a specific performance using properties prediction models¹⁵⁴. CAMD tools are widely used for the design of different applications, such as solvents^{155,156} and pharmaceuticals¹⁵⁷. In relation to those documents considering two or more types of products, a general interest in integrated methodologies is presented. An example of these is the grand model for chemical product design¹¹, which develops a framework containing methods, tools, databases, and procedures for the design of molecules, formulated products, devices, and functional products.

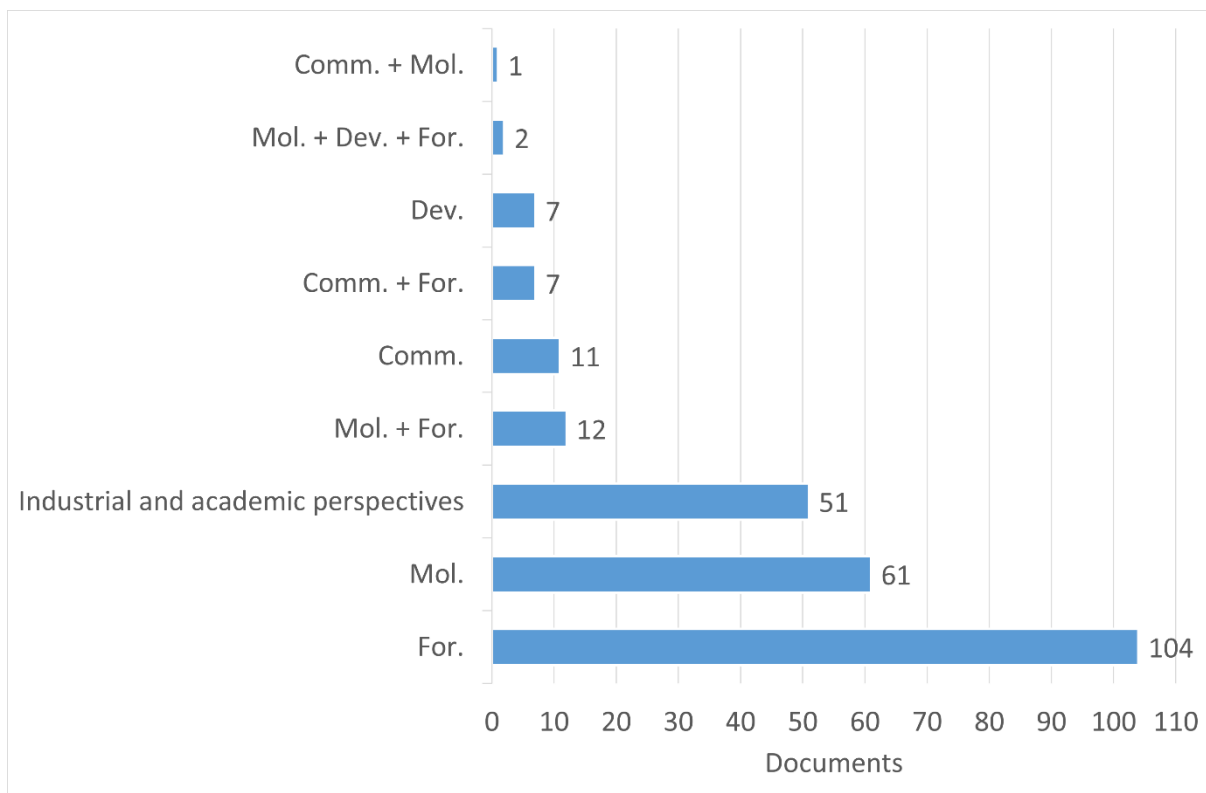


Figure 4. Classification of the documents retrieved from the bibliographic analysis and classified as highly relevant by type of chemical product mentioned in the methodology (Comm. = commodities, Mol. = molecules, Dev. = devices, For. = formulated)

An upward trend in the research output related to chemical product design methodologies may be highlighted in recent years. Figure 5 shows the cumulated mentions of each product type (including mentions of those documents which refer to more than one type of product): formulated (126), molecules (78), commodities (19), and devices (9). It is worth noting that in the evolution by product type, there is a marked interest in formulated products for the perspectives of product design in chemical engineering., as remarked by some authors ^{2,9}.

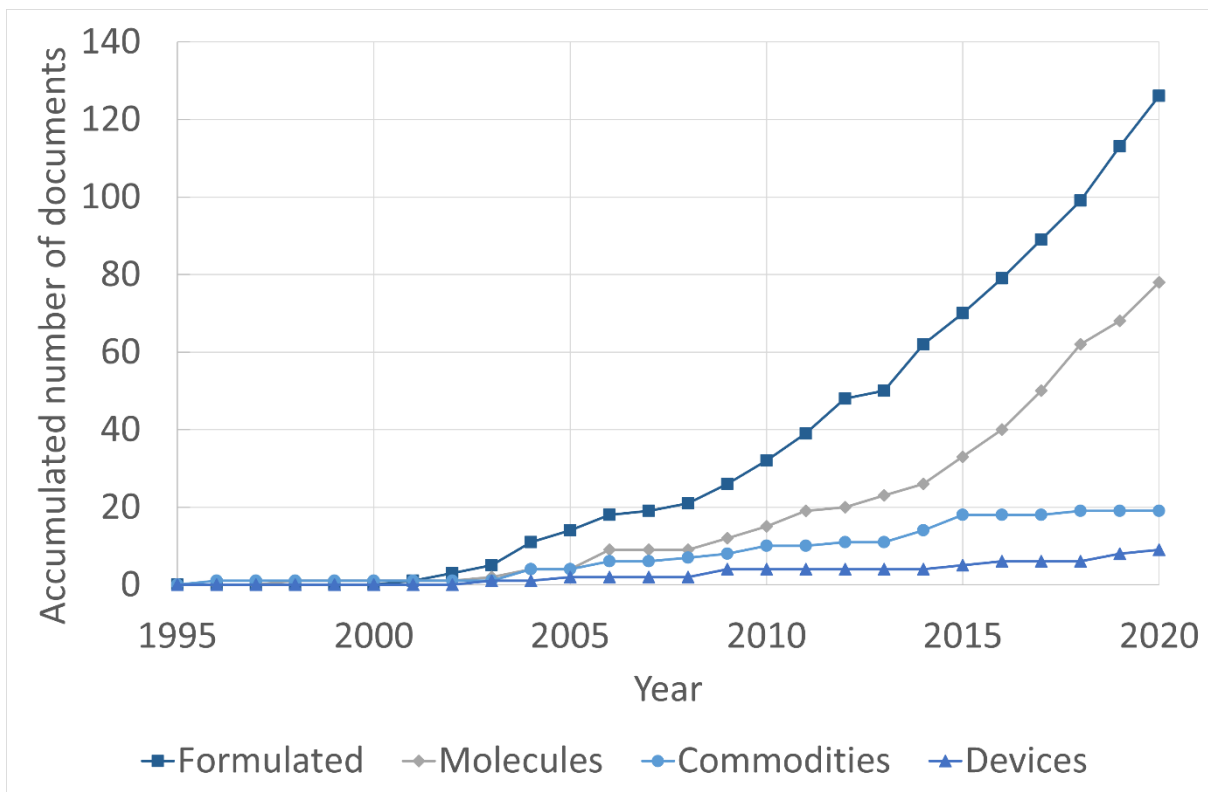


Figure 5. Accumulated product mention per year in scientific journals

Design phase

Figure 6 presents the publications classified by the design phases addressed in each document. The most frequently studied are the combination of the alternatives proposition and alternatives selection phases. For this group, there are 94 publications (44%). This shows that most product design methodologies focus on design problem solving by proposing a series of possible alternatives and subsequently assessing and ranking them according to their response to the design requirements. For example, in the approach presented by Jonuzaj et al.¹⁰³, a CAMD framework was applied in parallel with an optimization strategy. The framework enabled the proposition and selection of the best options according to target properties. The second most repeated combination is the one that includes the phases of needs analysis, alternatives proposition, and alternatives selection, with 24 publications (11%). These publications correspond to the methodologies addressing both problem definition and problem solving, where the customer needs become an important constraint for the design^{59,122,123}. Product design methodologies that include the process design phase are not commonly found in the documents despite the importance of the topic, especially for formulated products¹⁴³. In total (including mentions of those documents which refer to more than one design phase) there are 34 mentions of the process design phase in relation to chemical product design within the reviewed articles. This is a relatively low number compared to the phases of alternatives proposition (178 mentions) and alternatives selection (179 mentions). concerning the phases of needs analysis and needs translation, researches are beginning to study them, with 58 mentions of the first and 20 of the second, but not sufficiently, overall considering that most formulated products are consumer products.

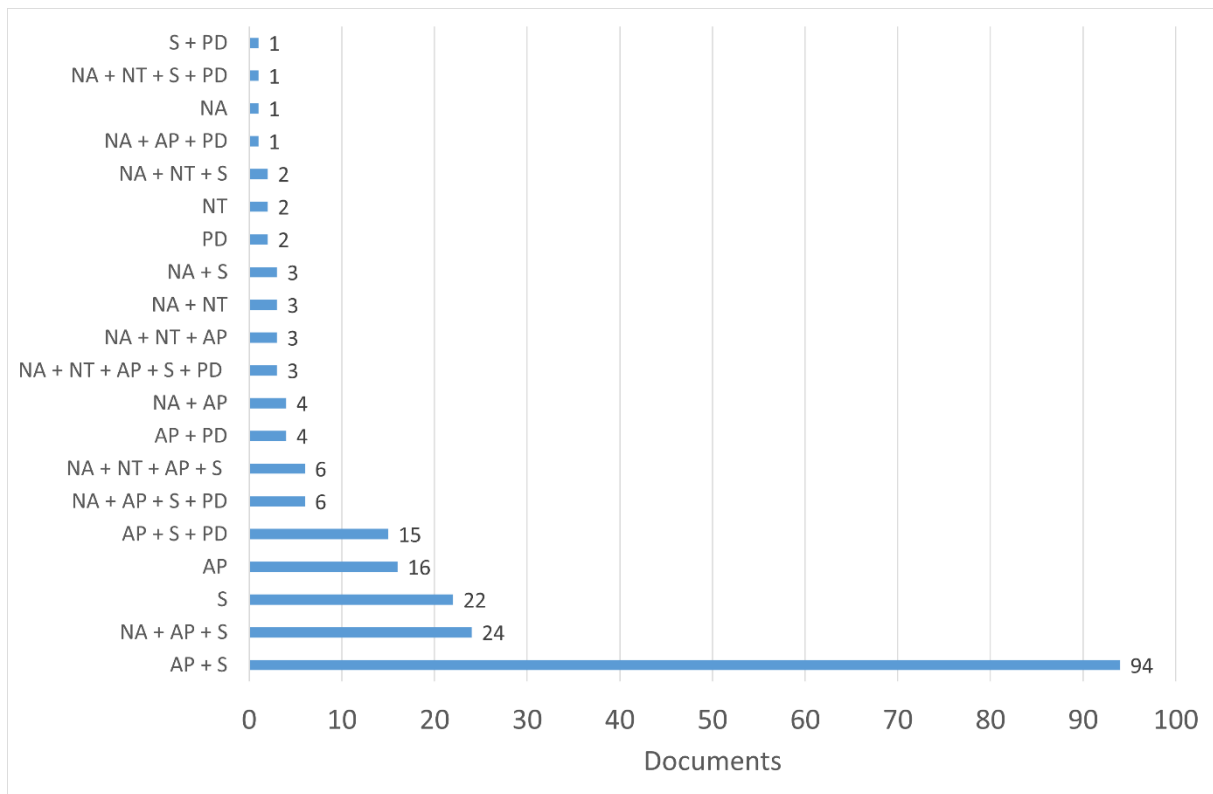


Figure 6. Classification of scientific journal documents by design phase (NA = needs analysis, NT = needs translation, AP = alternatives proposition, S = selection, PD = process design)

The integration of business approach in chemical product design

Figure 7 presents articles classified by product type and business approach. Articles containing a business approach are those which mention variables related to the company, its structure and functioning, e.g., articles that consider financial, marketing, production, and management aspects, among others. Figure 7 also presents publications that in addition to the business approach also consider the business strategy of the company where the methodology is applied, i.e., the value proposition is reflected in the design process, then the decision-making process is based on a business strategy. As presented in Figure 7, the business approach is rarely applied in chemical product design methodologies. Only 43 of the 257 publications reviewed (17%) take this aspect into account. It is noteworthy that the design methodologies which are classified as having a business approach currently integrate into their design process some variables related to the financial⁹⁹ or marketing aspects⁵⁷. As highlighted in Figure 7, the methodologies for formulated products pay more attention to the business context in comparison to other product types. Companies' interest in formulated products is used as a way to get into higher value-added markets¹³⁰. Design methodologies that integrate business elements into their decision-making process seem to present holistic visions. They embrace additional dimensions such as supply chains⁵² and government policies¹²⁶. In the publications where the design methodologies also integrate the business strategy (12 articles), the notion of an internal organizational structure appears^{1,11,144}. This notion is key to a design process that distinguishes operational, tactical, and strategic decisions.

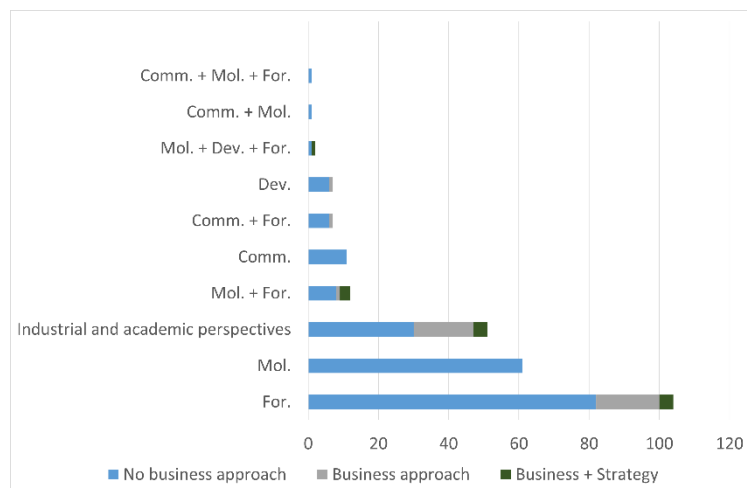


Figure 7. Classification of scientific journal documents by enterprise approach according to product type (Comm. = commodities, Mol. = molecules, Dev. = devices, For. = formulated)

Publications that mention formulated products were classified by industrial sector, as shown in Figure 8. The majority of the products developed in the documents reviewed correspond to applications of the type used in the business-to-business market, such as paints ¹³¹ or inks ¹⁰⁶ (50 articles out of 126). Generally, for that kind of product, specifications are well defined in technical terms, which is the reason why they may be preferred for validating design methodologies focused on alternatives proposition and selection. Moreover, regulations are more precise in these domains. Second-ranked products are cosmetics, with 25 publications out of 126. The methodologies concerning this industry pose a major challenge because it needs to be taken into account that the final properties of the products must respond to customer needs ⁵⁹.

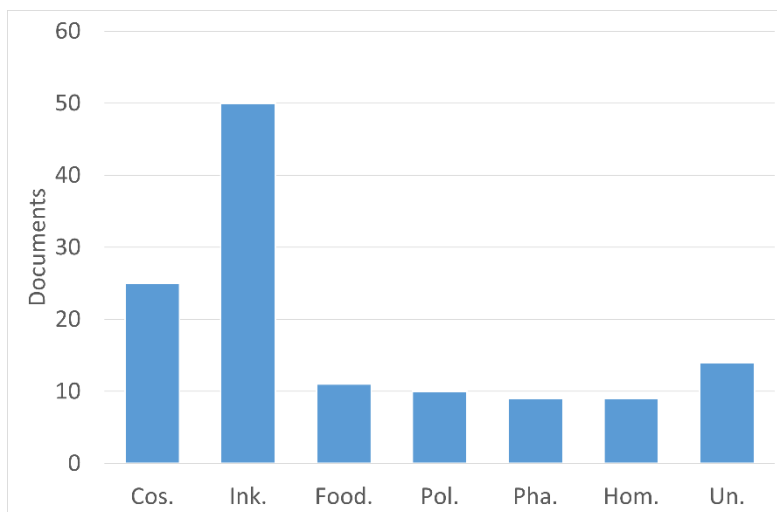


Figure 8. Formulated products classified by industrial application for the scientific journal documents (Cos. = cosmetics, Pha. = pharmaceuticals, Pol. = polymers and materials, Food. = food industry, Hom. = homecare, Ink. = solvents-fluids-paints-inks, Un. = unspecified)

PATENTS

Given the nature of the patents, the analysis procedure could not be carried out in the same way as before. Figure 9 shows the four categories identified in the analysis of patents: new product; new process; packaging or applicators; and product customization.

The patents show the recent developments in the industry, the interest in them, and the opportunities for innovation. Most of the patents correspond to the design of new products (44%) and processes (18%), which are the same aspects addressed in the design methodologies proposed by the academy. Interestingly, there are several patents in the packaging (11%), which, although not the majority, is significant. Packaging is an aspect that is completely disregarded in the methodologies reviewed, but it seems to be important in industrial practices. A methodology considering the simultaneous design of the product itself and its packaging may be an interesting research study with a direct application in the industry context. Such a methodology should consider how the company develops its design projects, how it is organized, and how information is shared between design actors. Moreover, Figure 9 also shows the existence of patents for customization (7%), a trend requiring high design capacity and innovation capability, specific forms of organization, and flexible working methods within the companies. For example, some invention patents correspond to a methodology for the product individualization of Shiseido ¹⁵⁸, a large Japanese cosmetics company where devices are proposed to evaluate sensory needs and algorithms are implemented to recommend product alternatives according to the expectations and requirements of the user.

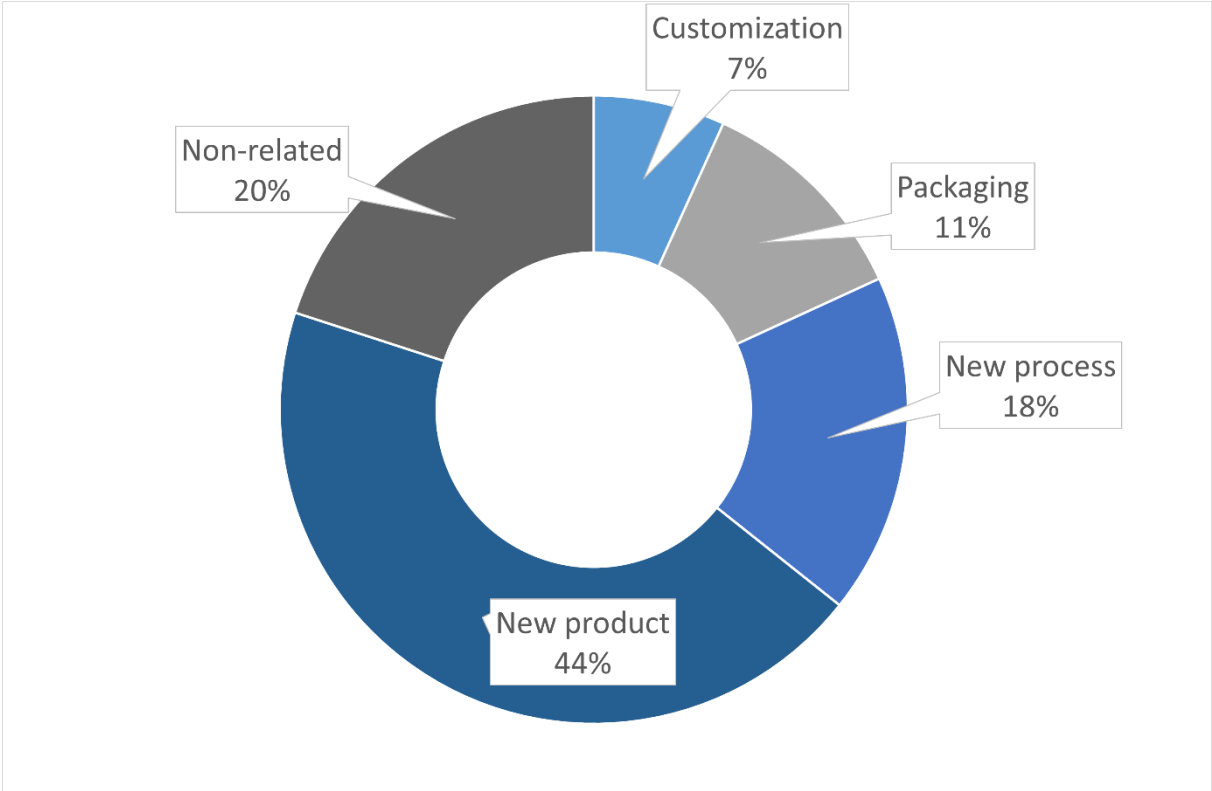


Figure 9. Percentage of documents in patent form by category

DISCUSSION AND PERSPECTIVES

Based on the previous bibliographic analysis, it is possible to identify the research directions explored until now within the field of Chemical Product Design. Figure 5 shows an evolution of the subject, where it is possible to evidence the increasing, and relatively recent interest in developing design methodologies specially for molecules and formulated products. Most of the published methodologies for both types of products apply a reverse design approach (to go from the properties or product specifications to the product). In that approach, product alternatives are generated with computer-aided methods based on thermodynamic modeling of properties, and best alternatives are subsequently selected, with consideration for dissimilar constraints through Mixed-Integer Nonlinear Programming algorithms^{136,159}. These methodologies have the same vision as those traditionally developed for process design in chemical engineering, where thermodynamics and transport phenomena have been the guiding thread.

Additionally, it has been widely accepted that chemical product design requires a multidisciplinary and multiscale approach. Product functional properties are determined at the nano- and micro-scales¹⁶⁰, the production process is defined at the meso- and macro-scales¹⁶¹, and product interactions with the users, the company, other stakeholders, and the environment occur at the mega-scale¹⁶². Thus, the design of products requires the inclusion of multiple aspects, such as thermodynamics, marketing, customer needs, business organization, sustainability, territoriality, and the supply chain, among others.

According to the bibliographic analysis, some proposals for product design methodologies are beginning to move slowly beyond the physicochemical reality of the product toward a multidisciplinary view of it, which includes the consideration of aspects such as customer needs and the business context. Customer needs connect the product with the reality of its use; while the business context refers to the interrelation of the product with the company and thus with the background in which it is developed by a design team. Some recent methodologies include business, marketing, and environmental issues. For example, there are design methodologies that include financial and marketing models in global product design approaches such as those proposed by¹⁰ and¹²⁶, among others. Though some interest in this direction, the number of publications including the business context within their design methodologies is still low (17%), which partly explains the difficulty of adapting the proposed product design methodologies to solve practical industrial problems¹⁶. This is similar in the case of the inclusion of user needs in the published methodologies: only 22% of them consider the phases of customer need analysis and 8% of them the phase of

customer needs translation. In these two stages the concept of the product is created and many decisions affecting the result are made.

In conclusion, concerning the aspects of business approach and customer needs, it became evident that there is currently no methodology that explores them in their full depth, at least in the case of formulated products. While most of the chemical design methodologies consider all or part of the design phases proposed by Cussler¹⁷, only a small portion of these methodologies consider that corporate strategy influences the decision-making process. On the one hand, works that include hierarchical methodologies for companies' decision-making regarding the design of formulated chemical products were found^{1,130}. On the other hand, multiple studies summarize their approaches to company decision-making based on a product cost function^{99,123}. Thus, the need for a common basis for chemical product design within a business context is visible. Such a basis would compile, among other things, technical aspects of the product, its properties conferred by its formulation, the needs of users and other stakeholders, and the development of business units. In addition, other aspects, such as the supply chain¹⁵² and government policies¹²⁶, which are useful as facilitators and/or constraints in the early stages of product design, should also be considered. In addition, the training of future chemical product designers must also include the development of interdisciplinary and business skills to allow them to be more context-aware, flexible and creative to meet today's product design challenges.

Finally, it is worth to highlight that the context where the design process takes place should be included in the new methodologies proposed for the design of formulated chemical products, because companies that develop that task must manage a complex challenge. To success in that challenge, the interdisciplinary team of the company involved in the design must work to solve technological, financial, economic, environmental, and social issues through the development of individual and collective tasks. In addition, each decision made by the interdisciplinary team, i. e. the selection of ingredients of the products and the simultaneous definition of the production process stages and operation conditions, the design of the container and the product visual identity, among many other, will have direct impact in other activities developed by other different business units of the company, impacting the value creation for the company and other stakeholders. Thus, the product design process is beyond just technical and economic issues and must be in tight concordance with the strategic goals of the company and its ecosystem (context, resources, etc), as well as aligned with the needs of the customers and actors outside the company but involved with the product being designed. For such reasons, each product design project must be adjusted to the company where it is developed, considering its business model and resources.

CONCLUSION

In this paper, a systematic literature review of product design methodologies regarding business considerations was performed through the analysis of 257 research documents. It includes a general mapping of methodologies for chemical product design, with consideration given to the type of chemical products addressed, the design phases developed, and how widely the existing methodologies include business aspects. From these results, it became evident that there is significant interest in the development of design methodologies that address the above-mentioned category of formulated products. Regarding the product design phases that the analyzed methodologies entail, there is significant demand for the development of design processes that integrate needs analysis as a fundamental basis for design, as well as completely integrated methodologies. In general, it is observed that in the methodologies analyzed, there is a lack of approaches that include a business-based context in their design process. Finally, it is also highlighted that interdisciplinary skills are required when executing a chemical product design project, which should therefore be viewed as an issue of increasing importance in the training of professionals.

REFERENCES

1. Heintz J, Belaud JP, Gerbaud V. Chemical enterprise model and decision-making framework for sustainable chemical product design. *Comput Ind.* 2014;65(3):505-520. doi:10.1016/j.compind.2014.01.010
2. Uhlemann J, Costa R, Charpentier JC. Product Design and Engineering in Chemical Engineering: Past, Present State, and Future. *Chem Eng Technol.* 2019;42(11):2258-2274. doi:10.1002/ceat.201900236
3. Filipovic M, Lukic M, Djordjevic S, et al. Towards satisfying performance of an O/W cosmetic emulsion: screening of reformulation factors on textural and rheological properties using general experimental design. *Int J Cosmet Sci.* 2017;39(5):486-499. doi:10.1111/ics.12402
4. Martín M, Martínez A. A methodology for simultaneous process and product design in the formulated consumer products industry: The case study of the detergent business. *Chem Eng Res Des.* 2013;91(5):795-809. doi:10.1016/j.cherd.2012.08.012
5. Šimberová I, Kita P. New business models based on multiple value creation for the customer: A case study in the chemical industry. *Sustain.* 2020;12(9):1-18. doi:10.3390/su12093932
6. Cooper RG. The drivers of success in new-product development. *Ind Mark Manag.* 2019;76(January 2018):36-47. doi:10.1016/j.indmarman.2018.07.005
7. Wang H, Chen K, Zheng H, Zhang G, Wu R, Yu X. Knowledge transfer methods for expressing product design information and organization. *J Manuf Syst.* 2021;58(PA):1-15. doi:10.1016/j.jmsy.2020.11.009
8. Kerm T Van, Noël L, Vêrilhac I. *Quand Le Design... s'investit Dans l'entreprise: 10 Entreprises Témoignent de l'impact Du Design Sur Leur Développement.* CITE DU DE.; 2012.
9. Arrieta-Escobar JA, Camargo M, Morel L, Orjuela A. Current approaches on chemical product design: A study of opportunities identification for integrated methodologies. In: *Towards the Digital World and Industry X.0 - Proceedings of the 29th International Conference of the International Association for Management of Technology, IAMOT 2020.* ; 2020:785-794.
10. Ng KM. MOPSD: a framework linking business decision-making to product and process design. *Comput Chem Eng.* 2004;29(1):51-56. doi:10.1016/j.compchemeng.2004.07.029

11. Fung KY, Ng KM, Zhang L, Gani R. A grand model for chemical product design. *Comput Chem Eng*. 2016;91:15-27. doi:10.1016/j.compchemeng.2016.03.009
12. Smith B V., Ierapepritou MG. Integrative chemical product design strategies: Reflecting industry trends and challenges. *Comput Chem Eng*. 2010;34(6):857-865. doi:10.1016/j.compchemeng.2010.02.039
13. Narvaez PC. *Diseño Conceptual de Procesos Químicos - Metodología Con Aplicaciones En Esterificación*. UNIVERSIDAD NACIONAL DE COLOMBIA; 2014. https://books.google.fr/books/about/Diseño_conceptual_de_procesos_químicos.html?id=SjGDwAAQBAJ&printsec=frontcover&source=kp_read_button&redir_esc=y#v=onepage&q&f=false. Accessed February 22, 2021.
14. Hill M. Chemical Product Engineering-The third paradigm. *Comput Chem Eng*. 2009;33(5):947-953. doi:10.1016/j.compchemeng.2008.11.013
15. Suárez Palacios OY, Narváez Rincón PC, Camargo M, et al. Chemical product design integrating MCDA: Performance prediction and human preferences modelling. *Can J Chem Eng*. 2020;(June 2020):1-15. doi:10.1002/cjce.23956
16. Zhang L, Mao H, Liu Q, Gani R. Chemical product design – recent advances and perspectives. *Curr Opin Chem Eng*. 2020;27:22-34. doi:10.1016/j.coche.2019.10.005
17. Cussler EL, Moggridge GD. *Chemical Product Design*. Vol 9780521168. Second.; 2011. doi:10.1017/CBO9781139035132
18. Ng LY, Andiappan V, Chemmangattuvalappil NG, Ng DKS. Novel methodology for the synthesis of optimal biochemicals in integrated biorefineries via inverse design techniques. *Ind Eng Chem Res*. 2015;54(21):5722-5735. doi:10.1021/acs.iecr.5b00217
19. Ho EN, Fung KY, Wibowo C, Zhang X, Ng KM. Conceptual design of chemical devices. *J Adv Manuf Process*. December 2020. doi:10.1002/amp2.10073
20. Chemmangattuvalappil NG, Eden MR. A Novel Methodology for Property-Based Molecular Design Using Multiple Topological Indices. *Ind Eng Chem Res*. 2013;52(22):7090-7103. doi:10.1021/ie302516v
21. Austin ND, Sahinidis N V., Trahan DW. Computer-aided molecular design: An introduction and review of tools, applications, and solution techniques. *Chem Eng Res Des*. 2016;116:2-26.

doi:10.1016/j.cherd.2016.10.014

22. Bardow A, Steur K, Gross J. Continuous-Molecular Targeting for Integrated Solvent and Process Design. *Ind Eng Chem Res.* 2010;49(6):2834-2840. doi:10.1021/ie901281w
23. Taifouris M, Martín M, Martínez A, Esquejo N. Challenges in the design of formulated products: multiscale process and product design. *Curr Opin Chem Eng.* 2020;27:1-9. doi:10.1016/j.coche.2019.10.001
24. Li X, Chen Y, Qian Y. Integration of chemical product development, process synthesis, and operation optimization. *Comput Aided Chem Eng.* 2009;26:37-42. doi:10.1016/S1570-7946(09)70009-4
25. Gani R, Ng KM. Product design - Molecules, devices, functional products, and formulated products. *Comput Chem Eng.* 2015;81:70-79. doi:10.1016/j.compchemeng.2015.04.013
26. Kontogeorgis GMGM, Mattei M, Ng KMKM, Gani R. An Integrated Approach for the Design of Emulsified Products. *AIChE J.* 2019;65(1):75-86. doi:10.1002/aic.16363
27. Calvo F, Gómez JM, Ricardez-Sandoval L, Alvarez O. Integrated design of emulsified cosmetic products: A review. *Chem Eng Res Des.* 2020;161:279-303. doi:10.1016/j.cherd.2020.07.014
28. Edwards MF. Product Engineering. *Chem Eng Res Des.* 2006;84(4):255-260. doi:10.1205/cherd05030
29. Chang S, Singh H. Corporate and industry effects on business unit competitive position. *Strateg Manag J.* 2000;21(7):739-752. doi:10.1002/1097-0266(200007)21:7<739::aid-smj117>3.3.co;2-h
30. Grossmann IE. Challenges in the new millennium: Product discovery and design, enterprise and supply chain optimization, global life cycle assessment. *Comput Chem Eng.* 2004;29(1):29-39. doi:10.1016/j.compchemeng.2004.07.016
31. Teece DJ. Business models, business strategy and innovation. *Long Range Plann.* 2010;43(2-3):172-194. doi:10.1016/j.lrp.2009.07.003
32. Casadesus-Masanell R, Ricart JE. From strategy to business models and onto tactics. *Long Range Plann.* 2010;43(2-3):195-215. doi:10.1016/j.lrp.2010.01.004

33. LOréal. *Annual Report 2018 - L'Oréal.*; 2018. https://www.loreal-finance.com/en/annual-report-2018/LOreal_2018_Annual_Report.pdf.
34. Smith B V., Ierapeprou MG. Modeling and optimization of product design and portfolio management interface. *Comput Chem Eng.* 2011;35(11):2579-2589.
doi:10.1016/j.compchemeng.2011.06.009
35. Wibowo C, Ng KM. Product-oriented process synthesis and development: Creams and pastes. *AIChE J.* 2001;47(12):2746-2767. doi:10.1002/aic.690471214
36. Wibowo C, Ng KM. Product-centered processing: Manufacture of chemical-based consumer products. *AIChE J.* 2002;48(6):1212-1230. doi:10.1002/aic.690480609
37. Rähse W, Hoffmann S. Produkt-Design – Zusammenwirken von Chemie, Technik und Marketing im Dienste des Kunden. *Chemie Ing Tech.* 2002;74(9):1220-1229.
doi:10.1002/1522-2640(20020915)74:9<1220::AID-CITE1220>3.0.CO;2-Z
38. Fung KY, Ng KM. Product-centered processing: Pharmaceutical tablets and capsules. *AIChE J.* 2003;49(5):1193-1215. doi:10.1002/aic.690490512
39. Rähse W, Hoffmann S. Product Design– The Interaction between Chemistry, Technology and Marketing to Meet Customer Needs. *Chem Eng Technol.* 2003;26(9):931-940.
doi:10.1002/ceat.200306106
40. Ng KM. MOPSD: A framework linking business decision-making to product and process design. In: ; 2003:63-73. doi:10.1016/S1570-7946(03)80527-8
41. Meyer TH, Keurentjes JTF. Polymer Reaction Engineering, an Integrated Approach. *Chem Eng Res Des.* 2004;82(12):1580-1582. doi:10.1205/cerd.82.12.1580.58035
42. Bernardo FP, Saraiva PM. Value of information analysis in product/process design. In: ; 2004:151-156. doi:10.1016/S1570-7946(04)80091-9
43. Abildskov J, Kontogeorgis GM. Chemical Product Design: A new challenge of applied thermodynamics. *Chem Eng Res Des.* 2004;82(11):1505-1510.
doi:10.1205/cerd.82.11.1505.52036
44. Hill M. Product and process design for structured products. *AIChE J.* 2004;50(8):1656-1661.
doi:10.1002/aic.10293

45. Ng KM, Li J, Kwauk M. Process engineering research in China: A multiscale, market-driven approach. *AIChE J.* 2005;51(10):2620-2627. doi:10.1002/aic.10658
46. Muro-Suñé N, Munir A, Gani R, Bell G, Shirley I. A framework for product analysis: Modelling and design of release and uptake of pesticides. In: ; 2005:733-738. doi:10.1016/S1570-7946(05)80244-5
47. Bernardo FP, Saraiva PM. Integrated process and product design optimization: a cosmetic emulsion application. *Comput Aided Chem Eng.* 2005;20(C):1507-1512. doi:10.1016/S1570-7946(05)80093-8
48. Yu Q, Zhihui W, Yanbin J. Integration of chemical product development, process design and operation based on a kilo-plant*. *Prog Nat Sci.* 2006;16(6):600-606. doi:10.1080/10020070612330041
49. Perrot N, Ioannou I, Allais I, Curt C, Hossenlopp J, Trystram G. Fuzzy concepts applied to food product quality control: A review. *Fuzzy Sets Syst.* 2006;157(9):1145-1154. doi:10.1016/j.fss.2005.12.013
50. Qian Y, Wu Z, Jiang Y, Zhihui W, Yanbin J. Integration of Process Design and Operation for Chemical Product Development with Implementation of a Kilo-plant. In: *Computer Aided Chemical Engineering*. Vol 21. Computer Aided Chemical Engineering. Elsevier; 2006:600-606. doi:10.1016/S1570-7946(06)80175-6
51. Gong H, Ding X, Ma L. Genetic algorithm for optimization of tobacco-group formulas design. In: *The Proceedings of the Multiconference on "Computational Engineering in Systems Applications."* IEEE; 2006:1532-1536. doi:10.1109/CESA.2006.313558
52. Bagajewicz MJ. On the role of microeconomics, planning, and finances in product design. *AIChE J.* 2007;53(12):3155-3170. doi:10.1002/aic.11332
53. Feng T-J, Ma L-T, Ding X-Q, Yang N, Xiao X. Intelligent techniques for cigarette formula design. *Math Comput Simul.* 2008;77(5-6):476-486. doi:10.1016/j.matcom.2007.11.025
54. Costa R, Elliott P, Saraiva PM, Aldridge D, Moggridge GD. Development of Sustainable Solutions for Zebra Mussel Control Through Chemical Product Engineering. *Chinese J Chem Eng.* 2008;16(3):435-440. doi:10.1016/S1004-9541(08)60101-9
55. Bongers PMM, Almeida-Rivera C. *Product Driven Process Synthesis Methodology*. Vol 26.

Elsevier B.V.; 2009. doi:10.1016/S1570-7946(09)70039-2

56. Conte E, Morales-Rodriguez R, Gani R. The Virtual Product-Process Design Laboratory for Design and Analysis of Formulations. In: ; 2009:825-830. doi:10.1016/S1570-7946(09)70358-X
57. Cheng YS, Lam KW, Ng KM, Ko RKM, Wibowo C. An integrative approach to product development—A skin-care cream. *Comput Chem Eng.* 2009;33(5):1097-1113. doi:10.1016/j.compchemeng.2008.10.010
58. Conte E, Morales-Rodriguez R, Gani R. The Virtual Product-Process Design Laboratory as a Tool for Product Development. In: ; 2009:249-254. doi:10.1016/S1570-7946(09)70042-2
59. Smith B V., Ierapeprou M. Framework for Consumer-Integrated Optimal Product Design. *Ind Eng Chem Res.* 2009;48(18):8566-8574. doi:10.1021/ie900377e
60. Solvason CC, Chemmangattuvalappil NG, Eden MR. Multi-Scale Chemical Product Design using the Reverse Problem Formulation. In: ; 2010:1285-1290. doi:10.1016/S1570-7946(10)28215-9
61. Omidbakhsh N, Elkamel A, Duever TA, Reilly PM. Combining Design of Experiments Techniques, Connectionist Models, and Optimization for the Efficient Design of New Product Formulations. *Chem Prod Process Model.* 2010;5(1). doi:10.2202/1934-2659.1441
62. Omidbakhsh N, Duever TA, Elkamel A, Reilly PM. Systematic statistical-based approach for product design: Application to disinfectant formulations. *Ind Eng Chem Res.* 2010;49(1):204-209. doi:10.1021/ie900196u
63. Stelzer T, Ulrich J. Crystallization a tool for product design. *Adv Powder Technol.* 2010;21(3):227-234. doi:10.1016/j.appt.2010.04.006
64. Cheng YS, Ng KM, Wibowo C. Product Design: a Transdermal Patch Containing a Traditional Chinese Medicinal Tincture. *Ind Eng Chem Res.* 2010;49(10):4904-4913. doi:10.1021/ie901554s
65. Wu Z, Lei Li, Ming Pan. A experimental platform for process operation system based on data integration. In: *2010 2nd International Conference on Education Technology and Computer.* IEEE; 2010:V2-131-V2-135. doi:10.1109/ICETC.2010.5529420
66. Bagajewicz M, Hill S, Robben A, et al. Product design in price-competitive markets: A case study of a skin moisturizing lotion. *AIChE J.* 2011;57(1):160-177. doi:10.1002/aic.12242

67. Linehan S, Nizami SN, Bagajewicz M. On the Application of a Consumer Preference-Based Method for Designing Products To Wine Fermentation Monitoring Devices. *Chem Eng Commun.* 2010;198(2):255-272. doi:10.1080/00986445.2010.499833
68. Frenkel M. Thermophysical and thermochemical properties on-demand for chemical process and product design. *Comput Chem Eng.* 2011;35(3):393-402. doi:10.1016/j.compchemeng.2010.12.013
69. Conte E, Gani R, Malik TI. The virtual Product-Process Design laboratory to manage the complexity in the verification of formulated products. *Fluid Phase Equilib.* 2011;302(1-2):294-304. doi:10.1016/j.fluid.2010.09.031
70. Abildskov J, O'Connell JP. Molecular Thermodynamic Modeling and Design of Microencapsulation Systems for Drug Delivery. *J Chem Eng Data.* 2011;56(4):1229-1237. doi:10.1021/je1011218
71. Conte E, Gani R, Ng KM. Design of Formulated Products: A Systematic Methodology. *AIChE J.* 2011;57(9):2431-2449. doi:10.1002/aic.12458
72. Cholakov GS. Towards computer aided design of fuels and lubricants. *J Univ Chem Technol Metall.* 2011;46(3):217-236.
73. Picchioni F, Broekhuis A. Material properties and processing in chemical product design. *Curr Opin Chem Eng.* 2012;1(4):459-464. doi:10.1016/j.coche.2012.08.002
74. Conte E, Gani R, Cheng YSYS, Ng KM. Design of formulated products: Experimental component. *AIChE J.* 2012;58(1):173-189. doi:10.1002/aic.12582
75. Victoria Villeda J, Dahmen M, Hechinger M, Voll A, Marquardt W. Towards model-based design of biofuel value chains. *Curr Opin Chem Eng.* 2012;1(4):465-471. doi:10.1016/j.coche.2012.08.001
76. Warriar P, Sathyanarayana A, Patil D V., France S, Joshi Y, Teja AS. Novel heat transfer fluids for direct immersion phase change cooling of electronic systems. *Int J Heat Mass Transf.* 2012;55(13-14):3379-3385. doi:10.1016/j.ijheatmasstransfer.2012.02.063
77. Ariffin Kashinath SA, Abdul Manan Z, Hashim H, Wan Alwi SR. Design of green diesel from biofuels using computer aided technique. *Comput Chem Eng.* 2012;41:88-92. doi:10.1016/j.compchemeng.2012.03.006

78. Warriar P, Sathyanarayana A, Bazdar S, Joshi Y, Teja AS. Selection and Evaluation of Organosilicon Coolants for Direct Immersion Cooling of Electronic Systems. *Ind Eng Chem Res.* 2012;51(31):10517-10523. doi:10.1021/ie300664v
79. Omidbakhsh N, Duever TA, Elkamel A, Reilly PM. A Systematic Computer-Aided Product Design and Development Procedure: Case of Disinfectant Formulations. *Ind Eng Chem Res.* 2012;51(45):14925-14934. doi:10.1021/ie300644f
80. Wassick JM, Agarwal A, Akiya N, Ferrio J, Bury S, You F. Addressing the operational challenges in the development, manufacture, and supply of advanced materials and performance products. *Comput Chem Eng.* 2012;47:157-169. doi:10.1016/j.compchemeng.2012.06.041
81. Samudra A, Sahinidis N V. Design of Heat-Transfer Media Components for Retail Food Refrigeration. *Ind Eng Chem Res.* 2013;52(25):8518-8526. doi:10.1021/ie303611v
82. Heintz J, Belaud J-P, Pandya N, Teles Dos Santos M, Gerbaud V. Computer aided product design tool for sustainable product development. *Comput Chem Eng.* 2014;71:362-376. doi:10.1016/j.compchemeng.2014.09.009
83. Santos J, Trujillo-Cayado LA, Calero N, Muñoz J. Physical characterization of eco-friendly O/W emulsions developed through a strategy based on product engineering principles. *AIChE J.* 2014;60(7):2644-2653. doi:10.1002/aic.14460
84. Ng LY, Chemmangattuvalappil NG, Ng DKS. A multiobjective optimization-based approach for optimal chemical product design. *Ind Eng Chem Res.* 2014;53(44):17429-17444. doi:10.1021/ie502906a
85. Bergez-Lacoste M, Thiebaud-Roux S, De Caro P, Fabre J-F, Gerbaud V, Mouloungui Z. From chemical platform molecules to new biosolvents: Design engineering as a substitution methodology. *Biofuels, Bioprod Biorefining.* 2014;8(3):438-451. doi:10.1002/bbb.1480
86. Mattei M, Kontogeorgis GM, Gani R. A comprehensive framework for surfactant selection and design for emulsion based chemical product design. *Fluid Phase Equilib.* 2014;362:288-299. doi:10.1016/j.fluid.2013.10.030
87. Tomba E, Barolo M, García-Muñoz S. In-silico product formulation design through latent variable model inversion. *Chem Eng Res Des.* 2014;92(3):534-544. doi:10.1016/j.cherd.2013.08.027

88. Ewoldt RH. Extremely Soft: Design with Rheologically Complex Fluids. *Soft Robot*. 2014;1(1):12-20. doi:10.1089/soro.2013.1508
89. Lee CKH, Choy KL, Chan YN. A knowledge-based ingredient formulation system for chemical product development in the personal care industry. *Comput Chem Eng*. 2014;65:40-53. doi:10.1016/j.compchemeng.2014.03.004
90. Yunus NA, Gernaey K V., Woodley JM, Gani R. A systematic methodology for design of tailor-made blended products. *Comput Chem Eng*. 2014;66:201-213. doi:10.1016/j.compchemeng.2013.12.011
91. Pavurala N, Achenie LEK. Identifying polymer structures for oral drug delivery – A molecular design approach. *Comput Chem Eng*. 2014;71:734-744. doi:10.1016/j.compchemeng.2014.07.015
92. Bernardo FP, Saraiva PM. A conceptual model for chemical product design. *AIChE J*. 2015;61(3):802-815. doi:10.1002/aic.14681
93. Azmin SN, Yunus NA, Mustaffa AA, Wan Alwi SR, Chua LS. A framework for solvent selection based on herbal extraction process design. *J Eng Sci Technol*. 2015;10(October 2017):25-34.
94. Victoria Villeda JJ, Dahmen M, Hechinger M, Voll A, Marquardt W. Towards Model-Based Design of Tailor-Made Fuels from Biomass. In: ; 2015:193-211. doi:10.1007/978-3-662-45425-1_12
95. Chong FK, Foo DCY, Eljack FT, Atilhan M, Chemmangattuvalappil NG. Ionic liquid design for enhanced carbon dioxide capture by computer-aided molecular design approach. *Clean Technol Environ Policy*. 2015;17(5):1301-1312. doi:10.1007/s10098-015-0938-5
96. Martín M, Martínez A. Addressing Uncertainty in Formulated Products and Process Design. *Ind Eng Chem Res*. 2015;54(22):5990-6001. doi:10.1021/acs.iecr.5b00792
97. Abdul Rahim Z, Lim Sing Sheng I, Nooh AB. TRIZ methodology for applied chemical engineering: A case study of new product development. *Chem Eng Res Des*. 2015;103:11-24. doi:10.1016/j.cherd.2015.08.027
98. Fatoni R, Elkamel A, Simon L, Almansoori A. A computer-aided framework for product design with application to wheat straw polypropylene composites. *Can J Chem Eng*. 2015;93(12):2141-2149. doi:10.1002/cjce.22346

99. Cheng YS, Fung KY, Ng KM, Wibowo C. Economic analysis in product design - A case study of a TCM dietary supplement. In: *Chinese Journal of Chemical Engineering*. Vol 24. ; 2016:202-214. doi:10.1016/j.cjche.2015.06.014
100. Chong FK, Foo DCY, Eljack FT, Atilhan M, Chemmangattuvalappil NG. A systematic approach to design task-specific ionic liquids and their optimal operating conditions. *Mol Syst Des Eng*. 2016;1(1):109-121. doi:10.1039/C5ME00013K
101. Dahmen M, Marquardt W. Model-Based Design of Tailor-Made Biofuels. *Energy & Fuels*. 2016;30(2):1109-1134. doi:10.1021/acs.energyfuels.5b02674
102. Austin ND, Samudra AP, Sahinidis N V., Trahan DW. Mixture design using derivative-free optimization in the space of individual component properties. *AIChE J*. 2016;62(5):1514-1530. doi:10.1002/aic.15142
103. Jonuzaj S, Akula PT, Kleniati P, Adjiman CS. The formulation of optimal mixtures with generalized disjunctive programming: A solvent design case study. *AIChE J*. 2016;62(5):1616-1633. doi:10.1002/aic.15122
104. Tam SK, Fung KY, Poon GSH, Ng KM. Product design: Metal nanoparticle-based conductive inkjet inks. *AIChE J*. 2016;62(8):2740-2753. doi:10.1002/aic.15271
105. Kiskini A, Zondervan E, Wierenga PA, Poiesz E, Gruppen H. Using product driven process synthesis in the biorefinery. *Comput Chem Eng*. 2016;91:257-268. doi:10.1016/j.compchemeng.2016.03.030
106. Chong FK, Eljack FT, Atilhan M, Foo DCY, Chemmangattuvalappil NG. A systematic visual methodology to design ionic liquids and ionic liquid mixtures: Green solvent alternative for carbon capture. *Comput Chem Eng*. 2016;91:219-232. doi:10.1016/j.compchemeng.2016.04.006
107. Alvarez O. Integrating creativity in the design of chemical products. In: *2017 Research in Engineering Education Symposium, REES 2017*. ; 2017:1-9.
108. Wan Qi W, Lik Yin N, Sivaneswaran U, Chemmangattuvalappil NG. A Novel Methodology for Molecular Design via Data Driven Techniques. *J Phys Sci*. 2017;28(Suppl. 1):1-24. doi:10.21315/jps2017.28.s1.1
109. Khor SY, Liam KY, Loh WX, et al. Computer Aided Molecular Design for alternative sustainable

- solvent to extract oil from palm pressed fibre. *Process Saf Environ Prot.* 2017;106:211-223.
doi:10.1016/j.psep.2017.01.006
110. Frutiger J, Cignitti S, Abildskov J, Woodley J, Sin G. Computational working fluid design under property uncertainties: Application to organic rankine cycle. In: *30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, ECOS 2017.* ; 2017.
111. Yang Y, Zou X, Xiao F, Dong H. Integrated product-process design approach for polyethylene production. *Chem Eng Trans.* 2017;61(2014):1009-1014. doi:10.3303/CET1761166
112. Jonuzaj S, Adjiman CS. Designing optimal mixtures using generalized disjunctive programming: Hull relaxations. *Chem Eng Sci.* 2017;159:106-130. doi:10.1016/j.ces.2016.08.008
113. Dahmen M, Marquardt W. Model-Based Formulation of Biofuel Blends by Simultaneous Product and Pathway Design. *Energy & Fuels.* 2017;31(4):4096-4121.
doi:10.1021/acs.energyfuels.7b00118
114. Holmes AM, Charlton A, Derby B, Ewart L, Scott A, Shu W. Rising to the challenge: applying biofabrication approaches for better drug and chemical product development. *Biofabrication.* 2017;9(3):033001. doi:10.1088/1758-5090/aa7bbd
115. Zhang L, Fung KY, Zhang X, Fung HK, Ng KM. An integrated framework for designing formulated products. *Comput Chem Eng.* 2017;107:61-76.
doi:10.1016/j.compchemeng.2017.05.014
116. Hada S, Herring RH, Eden MR. Mixture formulation through multivariate statistical analysis of process data in property cluster space. *Comput Chem Eng.* 2017;107:26-36.
doi:10.1016/j.compchemeng.2017.06.017
117. Kashinath SAA, Hashim H, Yunus NA, Mustaffa AA. Design of surfactant for water in diesel emulsion fuel for designing eco-friendly fuel. *Chem Eng Trans.* 2018;63(2006):433-438.
doi:10.3303/CET1863073
118. Martín M, Martínez A. On the effect of price policies in the design of formulated products. *Comput Chem Eng.* 2018;109:299-310. doi:10.1016/j.compchemeng.2017.11.019
119. Cignitti S, Mansouri SS, Woodley JM, Abildskov J. Systematic Optimization-Based Integrated Chemical Product–Process Design Framework. *Ind Eng Chem Res.* 2018;acs.iecr.7b04216.

doi:10.1021/acs.iecr.7b04216

120. Serna J, Boly V, Rincon PCN, Falk V. Improving knowledge capitalization in product formulation: A cosmetic industry study case. In: *Towards Sustainable Technologies and Innovation - Proceedings of the 27th Annual Conference of the International Association for Management of Technology, IAMOT 2018.* ; 2018:1-7.
121. Zhang L, Kalakul S, Liu L, Elbashir NO, Du J, Gani R. A Computer-Aided Methodology for Mixture-Blend Design. Applications to Tailor-Made Design of Surrogate Fuels. *Ind Eng Chem Res.* 2018;57(20):7008-7020. doi:10.1021/acs.iecr.8b00775
122. Derkyi NSA, Acheampong MA, Mwin EN, Tetteh P, Aidoo SC. Product design for a functional non-alcoholic drink. *South African J Chem Eng.* 2018;25:85-90.
doi:10.1016/j.sajce.2018.02.002
123. Chan YC, Fung KY, Ng KM. Product design: A pricing framework accounting for product quality and consumer awareness. *AIChE J.* 2018;64(7):2462-2471. doi:10.1002/aic.16153
124. Zhang L, Mao H, Liu L, Du J, Gani R. A machine learning based computer-aided molecular design/screening methodology for fragrance molecules. *Comput Chem Eng.* 2018;115:295-308. doi:10.1016/j.compchemeng.2018.04.018
125. Kalakul S, Zhang L, Fang Z, et al. Computer aided chemical product design – ProCAPD and tailor-made blended products. *Comput Chem Eng.* 2018;116:37-55.
doi:10.1016/j.compchemeng.2018.03.029
126. Zhang X, Zhang L, Fung KY, Rangaiah GP, Ng KM. Product design: Impact of government policy and consumer preference on company profit and corporate social responsibility. *Comput Chem Eng.* 2018;118:118-131. doi:10.1016/j.compchemeng.2018.06.026
127. Arrieta-Escobar JA, Bernardo FP, Orjuela A, Camargo M, Morel L. Incorporation of heuristic knowledge in the optimal design of formulated products: Application to a cosmetic emulsion. *Comput Chem Eng.* 2019;122:265-274. doi:10.1016/j.compchemeng.2018.08.032
128. Frutiger J, Cignitti S, Abildskov J, Woodley JM, Sin G. Computer-aided molecular product-process design under property uncertainties – A Monte Carlo based optimization strategy. *Comput Chem Eng.* 2019;122:247-257. doi:10.1016/j.compchemeng.2018.08.021
129. Lee CKHKH. A knowledge-based product development system in the chemical industry. *J Intell*

Manuf. 2017;1-16. doi:10.1007/s10845-017-1331-5

130. Lai YY, Yik KCH, Hau HP, Chow CP, Chemmangattuvalappil NG, Ng LY. Enterprise Decision-making Framework for Chemical Product Design in Integrated Biorefineries. *Process Integr Optim Sustain.* 2019;3(1):25-42. doi:10.1007/s41660-018-0037-2
131. Rafeqah R, Hassim MH, Denny NKS, Nishanth GC, Norafneeza N. Safety and health index development for formulated product design: Paint formulation. Abd Jalil A, ed. *E3S Web Conf.* 2019;90:03002. doi:10.1051/e3sconf/20199003002
132. Jhamb S, Liang X, Gani R, Kontogeorgis GM. Systematic Model-Based Methodology for Substitution of Hazardous Chemicals. *ACS Sustain Chem Eng.* 2019;7(8):7652-7666. doi:10.1021/acssuschemeng.8b06064
133. Liu Q, Zhang L, Liu L, et al. OptCAMD: An optimization-based framework and tool for molecular and mixture product design. *Comput Chem Eng.* 2019;124:285-301. doi:10.1016/j.compchemeng.2019.01.006
134. Neoh JQ, Chin HH, Mah AXY, Aboagwa OA, Thangalazhy-Gopakumar S, Chemmangattuvalappil NG. Design of bio-oil additives using mathematical optimisation tools considering blend functionality and sustainability aspects. *Sustain Prod Consum.* 2019;19:53-63. doi:10.1016/j.spc.2019.03.005
135. Zhang X, Zhang L, Fung KY, Ng KM. Product design: Incorporating make-or-buy analysis and supplier selection. *Chem Eng Sci.* 2019;202:357-372. doi:10.1016/j.ces.2019.03.021
136. Liang X, Zhang X, Zhang L, et al. Computer-Aided Polymer Design: Integrating Group Contribution and Molecular Dynamics. *Ind Eng Chem Res.* 2019;58(34):15542-15552. doi:10.1021/acs.iecr.9b02769
137. Zhang X, Zhou T, Zhang L, Fung KY, Ng KM. Food Product Design: A Hybrid Machine Learning and Mechanistic Modeling Approach. *Ind Eng Chem Res.* 2019;58(36):16743-16752. doi:10.1021/acs.iecr.9b02462
138. Nelson AZ, Schweizer KS, Rauzan BM, Nuzzo RG, Vermant J, Ewoldt RH. Designing and transforming yield-stress fluids. *Curr Opin Solid State Mater Sci.* 2019;23(5):100758. doi:10.1016/j.cossms.2019.06.002
139. Jonuzaj S, Cui J, Adjiman CS. Computer-aided design of optimal environmentally benign

- solvent-based adhesive products. *Comput Chem Eng.* 2019;130:106518.
doi:10.1016/j.compchemeng.2019.106518
140. Torres JJ, Tinjaca CD, Alvarez OA, Gómez JM. Optimization proposal for emulsions formulation considering a multiscale approach. *Chem Eng Sci.* 2020;212:115326.
doi:10.1016/j.ces.2019.115326
141. Jhamb S, Liang X, Dam-Johansen K, Kontogeorgis GM. A model-based solvent selection and design framework for organic coating formulations. *Prog Org Coatings.* 2020;140:105471.
doi:10.1016/j.porgcoat.2019.105471
142. Cardona Jaramillo JEC, Achenie LE, Álvarez OA, Carrillo Bautista MP, González Barrios AF. The multiscale approach to the design of bio-based emulsions. *Curr Opin Chem Eng.* 2020;27:65-71. doi:10.1016/j.coche.2019.11.008
143. König A, Neidhardt L, Viell J, Mitsos A, Dahmen M. Integrated design of processes and products: Optimal renewable fuels. *Comput Chem Eng.* 2020;134:106712.
doi:10.1016/j.compchemeng.2019.106712
144. Marques CM, Moniz S, de Sousa JP, Barbosa-Povoa AP, Reklaitis G. Decision-support challenges in the chemical-pharmaceutical industry: Findings and future research directions. *Comput Chem Eng.* 2020;134:106672. doi:10.1016/j.compchemeng.2019.106672
145. Papadopoulos AI, Shavaliyeva G, Papadokostantakis S, et al. An approach for simultaneous computer-aided molecular design with holistic sustainability assessment: Application to phase-change CO₂ capture solvents. *Comput Chem Eng.* 2020;135:106769.
doi:10.1016/j.compchemeng.2020.106769
146. Chai S, Liu Q, Liang X, et al. A grand product design model for crystallization solvent design. *Comput Chem Eng.* 2020;135:106764. doi:10.1016/j.compchemeng.2020.106764
147. Cheng KC, Khoo ZS, Lo NW, Tan WJ, Chemmangattuvalappil NG. Design and performance optimisation of detergent product containing binary mixture of anionic-nonionic surfactants. *Heliyon.* 2020;6(5):e03861. doi:10.1016/j.heliyon.2020.e03861
148. Sunkle S, Saxena K, Patil A, et al. Information Extraction and Graph Representation for the Design of Formulated Products. In: *Lecture Notes in Computer Science (Including Subseries Lecture Notes in Artificial Intelligence and Lecture Notes in Bioinformatics)*. Vol 12127 LNCS. ;

2020:433-448. doi:10.1007/978-3-030-49435-3_27

149. Raslan R, Hassim MH, Chemmangattuvalappil NG, Ng DKS, Ten JY. Development of inherent safety and health index for formulated product design. *J Loss Prev Process Ind.* 2020;66:104209. doi:10.1016/j.jlp.2020.104209
150. Mushtaq F, Zhang X, Fung KY, Ng KM. Product design: An optimization-based approach for targeting of particulate composite microstructure. *Comput Chem Eng.* 2020;140:106975. doi:10.1016/j.compchemeng.2020.106975
151. Raslan R, Hassim MH, Chemmangattuvalappil NG, Ng DKS, Ten JY. Safety and health risk assessment methodology of dermal and inhalation exposure to formulated products ingredients. *Regul Toxicol Pharmacol.* 2020;116:104753. doi:10.1016/j.yrtph.2020.104753
152. Taifouris M, Martín M, Martínez A, Esquejo N. On the effect of the selection of suppliers on the design of formulated products. *Comput Chem Eng.* 2020;141:106980. doi:10.1016/j.compchemeng.2020.106980
153. Alshehri AS, Gani R, You F. Deep learning and knowledge-based methods for computer-aided molecular design—toward a unified approach: State-of-the-art and future directions. *Comput Chem Eng.* 2020;141:107005. doi:10.1016/j.compchemeng.2020.107005
154. Gertig C, Leonhard K, Bardow A. Computer-aided molecular and processes design based on quantum chemistry: current status and future prospects. *Curr Opin Chem Eng.* 2020;27:89-97. doi:10.1016/j.coche.2019.11.007
155. Chang SSL, Kong YL, Lim WX, Ooi J, Ng DKS, Chemmangattuvalappil NG. Design of alternate solvent for recovery of residual palm oil: simultaneous optimization of process performance with environmental, health and safety aspects. *Clean Technol Environ Policy.* 2018;20(5):949-968. doi:10.1007/s10098-018-1515-5
156. Rodriguez-Donis I, Thiebaud-Roux S, Lavoine S, Gerbaud V. Computer-aided product design of alternative solvents based on phase equilibrium synergism in mixtures. *Comptes Rendus Chim.* 2018;21(6):606-621. doi:10.1016/j.crci.2018.04.005
157. Houssein EH, Hosney ME, Oliva D, Mohamed WM, Hassaballah M. A novel hybrid Harris hawks optimization and support vector machines for drug design and discovery. *Comput Chem Eng.* 2020;133:106656. doi:10.1016/j.compchemeng.2019.106656

158. Ando S. METHOD FOR PROVIDING COSMETIC PRODUCT CUSTOMIZED FOR CUSTOMER. 2020. https://patentscope.wipo.int/search/es/detail.jsf?docId=WO2020194365&tab=PCTBIBLIO&_cid=P22-KI778W-46975-1.
159. Chávez-Islas LM, Vasquez-Medrano R, Flores-Tlacuahuac A. Optimal Molecular Design of Ionic Liquids for High-Purity Bioethanol Production. *Ind Eng Chem Res*. 2011;50(9):5153-5168. doi:10.1021/ie101791t
160. Kind M. Product engineering. *Chem Eng Process Process Intensif*. 1999;38(4-6):405-410. doi:10.1016/S0255-2701(99)00038-0
161. Costa R, Moggridge GD, Saraiva PM. Chemical product engineering: An emerging paradigm within chemical engineering. *AIChE J*. 2006;52(6):1976-1986. doi:10.1002/aic.10880
162. Cisternas LA. Nature of Chemical Products. In: Ng KM, Gani R, Dam-johansen K, eds. *Chemical Product Design: Towards a Perspective through Case Studies*. First Edit. Elsevier Science; 2006:459.