A system approach to support a methodology for the design of formulated cosmetic products in the context of companies

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Mentions: **Chemical engineering and Industrial Systems Engineering**

By:

Jose Luis Rivera Gil

Defended on December 14, 2022, in Nancy

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Doctor of Engineering – Chemical Engineering

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To Gael and Aron

“Even the smallest person can change the course of the future” J.R.R. Tolkien

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Resumen

Un enfoque de sistema para apoyar una metodología de diseño de productos cosméticos formulados en el contexto de las empresas.

Gestionar un proyecto de diseño y desarrollo de un nuevo producto químico es una tarea compleja a diferentes niveles. Además de los retos técnicos de la formulación y la definición de las condiciones del proceso, los equipos de diseño también deben tener en cuenta los requisitos de la organización donde se realiza el diseño del producto. Por lo tanto, en esta investigación se explora la dimensión organizativa y su importancia en el diseño de productos químicos. A través de una revisión bibliográfica, se encontró que las metodologías de diseño de productos químicos que integran el contexto organizacional no han sido analizadas a fondo y son altamente requeridas. En esta investigación, a través de un análisis sistémico basado en la información recopilada en entrevistas semiestructuradas con expertos en diseño del sector cosmético, se estudiaron las características del contexto organizacional y sus efectos en el proceso de diseño de productos de dicho sector. Además, la información capturada durante dichas entrevistas se formalizó en una base de conocimiento experto de recomendaciones para apoyar el proceso de diseño de productos cosméticos. Se propuso una herramienta para adaptar esas recomendaciones al proceso de diseño de empresas específicas. La herramienta se aplica a través de talleres colaborativos que permiten la participación activa del equipo de diseño en la evaluación del proceso de diseño para seleccionar e implementar las recomendaciones más adecuadas. Por último, la herramienta se aplica en una organización real mostrando cómo puede utilizarse para evaluar y mejorar un proceso de diseño real. En ese caso se comprobó que la herramienta propone soluciones de mejora adaptadas y alineadas con los conceptos de valor de la empresa, donde el equipo de diseño tiene el papel de evaluador y constructor de su propia metodología de diseño.

Palabras clave: Diseño de productos químicos, productos cosméticos, análisis de sistemas, contexto organizativo, metodología de diseño.

Résume

Une approche systémique pour supporter une méthodologie de conception de produits cosmétiques formules dans le contexte des entreprises.

La gestion d'un projet de conception et de développement d'un nouveau produit chimique est une tâche complexe à différents niveaux. En plus des défis techniques de la formulation et de la définition des conditions du processus, les équipes de conception doivent également prendre en compte les exigences de l'organisation dans laquelle la conception du produit est réalisée. Par conséquent, la dimension organisationnelle et son importance dans la conception de produits chimiques sont explorées dans cette recherche. Une revue bibliométrique de la littérature a permis de constater que les méthodologies de conception de produits chimiques intégrant le contexte organisationnel n'ont pas été analysées en profondeur et sont hautement nécessaires. Dans cette recherche, une analyse systémique basée sur les informations recueillies lors d'entretiens semi-structurés avec des experts en conception du secteur cosmétique a permis d'étudier les caractéristiques du contexte organisationnel et ses effets sur le processus de conception de produits de ce secteur. De plus, les informations recueillies lors de ces entretiens ont été formalisées dans une base de connaissances d'experts contenant des recommandations pour soutenir le processus de conception de produits cosmétiques. Un outil permettant d'adapter ces recommandations au processus de conception d'entreprises spécifiques a été proposé. L'outil est appliqué dans le cadre d'ateliers collaboratifs qui permettent la participation active de l'équipe de conception à l'évaluation du processus de conception afin de sélectionner et de mettre en œuvre les recommandations les plus appropriées. Enfin, l'outil est appliqué dans une organisation réelle montrant comment il peut être utilisé pour évaluer et améliorer un processus de conception réel. Dans ce cas, il a été constaté que l'outil propose des solutions d'amélioration adaptées et alignées sur les concepts de valeur de l'entreprise, où l'équipe de conception a le rôle d'évaluateur et de constructeur de sa propre méthodologie de conception.

Mots clés : Conception de produits chimiques, produits cosmétiques, analyse des systèmes, contexte organisationnel, méthodologie de conception.

Abstract

A system approach to support a methodology for the design of formulated cosmetic products in the context of companies

Managing a new chemical product design and development project is a complex task at different levels. In addition to the technical challenges of the formulation and the definition of process conditions, design teams should also consider the requirements of the organization where the product design is performed. Therefore, the organizational dimension and its importance in chemical product design are explored in this research. Through a bibliometric literature review, it was found that chemical product design methodologies integrating the organizational context have not been thoroughly analyzed and are highly required. In this research, through a systemic analysis based on information collected in semi-structured interviews with design experts of the cosmetic sector, the characteristics of the organizational context and its effects on the product design process of that sector were studied. Additionally, information captured during those interviews was formalized in an expert knowledge base of recommendations to support the cosmetic product design process. A tool to adapt those recommendations to the design process of specific companies was proposed. The tool is applied through collaborative workshops which enable the active participation of the design team in the evaluation of the design process in order to select and implement the most suitable recommendations. Finally, the tool is applied in a real organization showing how it can be used to evaluate and improve a real design process. In that case it was found that the tool proposes adapted improvement solutions aligned to the company's value concepts, where the design team has the role of evaluator and builder of its own design methodology.

Keywords: Chemical product design, cosmetic products, systems analysis, organizational context, design methodology

Content

List of Figures

Pág.

List of tables

Pág.

1 Introduction

1.1 General Context

Design problems can be as simple as finding a clear way to communicate a message or as complex as putting a satellite into orbit. The design process is both an individual and a collective human activity. On the individual side, it is a daily activity, which must respond to basic or highly complex problems. As a collective task, multidisciplinary groups confront their ideas, knowledge, and experience (Boly et al., 2016). Designing a product according to the C-K theory describes a process in which a designer thinks a new object by the interaction between the concept space and the knowledge space. In this process, the designer explores and imagines new concepts, and then he uses that knowledge to create objects and new concepts (Hatchuel & Weil, 2003).

For organizations, design of new products is fundamental to maintain or improve their competitive advantages in the market (Morel & Boly, 2006) . Design and product launch in organizations involve the activities of creating, developing, and marketing a product that is accepted by customers and satisfies their needs. Chemical companies face different situations and special challenges according to the type of product they are designing, considering the satisfaction and constraints of the market and the target customer they want to reach (Gani & Ng, 2015).

The importance of the chemical sector

The chemical industry reported a value of €3471 billion worldwide in 2022.The European Union accounted for about 14% of total sales, being second only to China which has 46% of total sales(CEFIC, 2022). The global value expected for 2030 is €6200 billion, which is a growth of 77% in only one decade. Figure 1-1 shows the market share of chemical products according to the product type categories for Europe in 2018. Consumer chemicals and specialty chemicals accounted for about 40% of total sales in Europe and present a major challenge in their design and commercialization when compared to commodity chemicals and petroleum products. The challenges of consumer chemicals and specialty chemicals emerges from the fact that these are products that respond to the demands framed by the final consumer, which react quickly to the dynamic trends of the global market, whereas these are products that take considerable time to design and develop given their technical, legal, safety, and performance requirements among others.

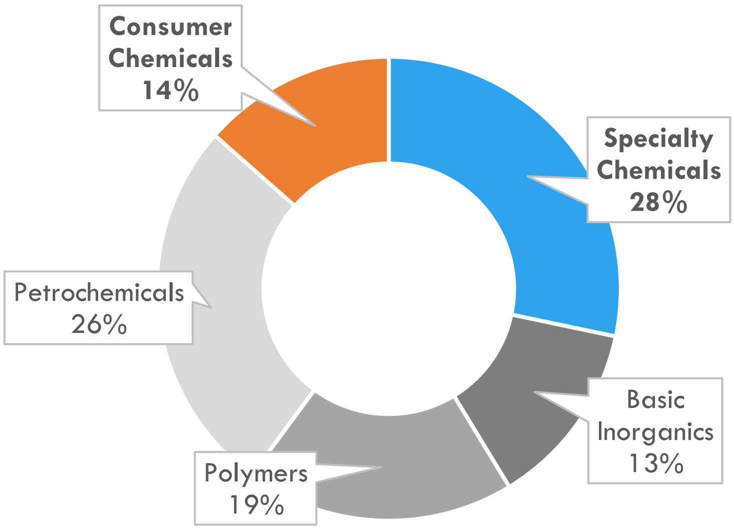

Figure 1-1: Participation of chemical sales by type of product in 2018 for the European Union c

Chemical industry has undergone a transition in recent decades, from commodities towards consumer chemical products. Figure 1-2 illustrates an example of that transformation, for the USA the workforce of the traditional chemical industry dedicated to the production of basic chemicals went from 75% of the total sector in 1975 to less than 25% in 2010. On the contrary, the jobs offered by the consumer chemicals industries went from being less than 15% to more than 50% for the same years (Cussler & Moggridge, 2011). This behavior creates the opportunity for new and old chemical companies to target markets that are more dynamic, demanding and competitive than the traditional markets in which commodity and petrochemical products are sold. In this context, companies are confronted to new business challenges when creating their products such as technical obstacles and market conditions.

Designing chemical products: the present context

When chemical companies design a new product, they must satisfactorily and harmoniously complete the requirements of the design considering at least three dimensions: technical, organizational and sustainable (Heintz, Belaud, & Gerbaud, 2014; Uhlemann et al., 2019). From a technical point of view, a synergistic action of the ingredients, their composition, and the manufacturing process confer the properties to the product. Thus, the combinations of these three type of variables can generate a huge solution space with multiple acceptable solutions (Filipovic et al., 2017; Martín & Martínez, 2013). From an organizational point of view, that large solution space should be limited in order to meet, not just user expectations, but also the requirements and desires of other stakeholders, particularly those of the organization where the product is created (Šimberová & Kita, 2020). In this regard, the product design process must be in alignment with the strategy and organizational plan of the company. Additionally, products must be designed following the principles of sustainability from different dimensions: social, economic, environmental, political, and technological (Narvaez, 2014). Sustainability performance of the organizations will be linked to the decisions made in the design and development stages of the product. Thus, the organizational context in which the product design activity takes place can constrain or influence the decisions made by design teams.

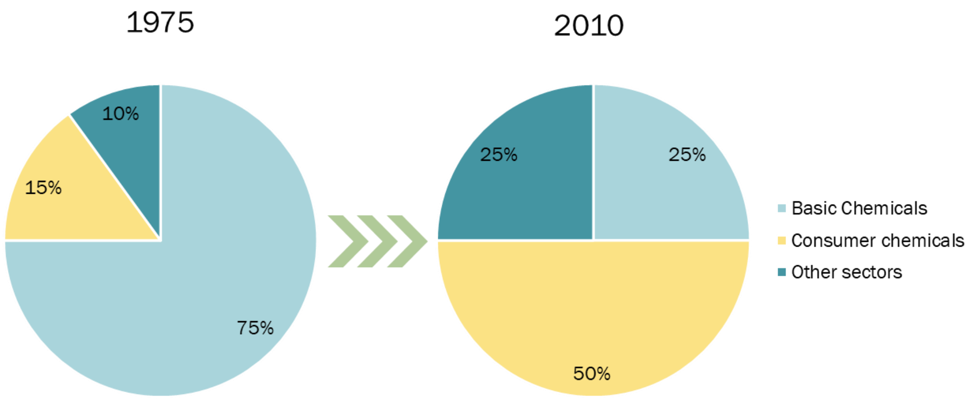

Figure 1-2 Distribution of employment in USA for the chemical industry for 1975 and 2010 (Cussler & Moggridge, 2011)

Formulation: a particular process

The design process for consumer chemical products from a includes at least, from an classical point of view, the following steps: (1) setting technical, organizational and sustainability objective, (2) the research of customer demands and their translation into technological specifications, (3) the conceptualization of the product, (4) the selection of raw materials and suppliers, (5) and the design of the production process (Cooper, 2019). It is a multi-objective, multi-stakeholder process that poses a significant challenge for businesses since they must manage information and knowledge related to all design variables throughout the whole product design and development cycle (Wang et al., 2021).

Furthermore, it is commonly acknowledged that chemical product design requires a multidisciplinary and multiscale approach (Cisternas, 2006; Costa et al., 2006; Kind, 1999) to consider physical properties, process design, and user-product interactions. Thus, product design involves the combination of several knowledge fields including thermodynamics, marketing, consumer needs, business organization, sustainability, territoriality, and supply chain, among others(Fung et al., 2016; L. Zhang et al., 2020).

Based on the above-mentioned aspects, one key characteristic to be addressed in this doctoral research is:

Organizational context: The organizational context for product design involves the interaction of multiple actors with different competencies and responsibilities(Goodwin, 2009). These actors can be internal to the organization, such as the project manager, design team, laboratory technician, quality manager, purchasing manager, among others. They can also be external, such as users, customers, suppliers, regulatory entities, or external consultants. The role of the actors and their interrelationships are specific to each company and are dynamic during the development of the design process. In this sense, design process it is a detailed activity that takes place in a complex and changing organizational context. Different approaches may be used depending on the company culture to respond to a similar design problem. In addition, the design process is not linear. It requires intermediate validations and multiple iteration cycles until the product can be launched on the market. Then, the success of a product depends not only on the correct selection of ingredients and the manufacturing process. While meeting technical requirements, it must also satisfy the expectations and requirements of stakeholders, notably the final user and others such as regulators, as well as less well-defined specifications, such as being in line with market and consumer trends.

The lack of the inclusion of organizational context in the design process, is a research opportunity for the proposition of a design tool that considers this aspect. Their analysis may enable to understand which are the key moments within a product design project, as well as to recognize the actors, and the decisions made in different levels from the corporate strategy to the product formulation.

1.2 Research scope and associated problems

To narrow down the scope of this research work and at the same time to further develop research lines of the laboratories and research groups involved in this work, this study is focused on the cosmetic industry. Products in this industry are aimed at the final consumer and most of the products are a good example of formulated chemicals. Cosmetics industries operate in a context of rapidly evolving markets and increasingly informed and demanding consumers (Suaza Montalvo, 2020). As a result, companies that design these types of chemical products must respond more quickly and accurately by launching new products on the market to survive in that very competitive environment.

Moreover, aspects involved in product design projects, such as creativity, innovation, multidisciplinary teamwork, decision making, ingredient selection, process design, scaling, launching, and selling, are carried out in an organizational context. Therefore, chemical product design methodologies must be aligned with the market in which they are been applied. According to our analysis of the state of the art (Chapter 2), chemical product design is a current topic that has attracted the attention of chemical engineering researchers. However, much of the scientific production in the area does not adequately represent the need to consider the real context of the design of chemical products: product design is performed in organizations and the outcome of the design is limited by the resources and capabilities of the organizations where it takes place.

Considering the above, this work addresses the following research question

How to design formulated chemical products considering the company context in the design process?

The hypothesis statement responding this research question reads as follows:

A design methodology for formulated chemical products, based on the analysis of the system created within the companies during a design project, will allow the design team to have a global perspective of the entire design process. This will allow the design team to make more informed decisions at early design stages and follow a less iterative design trajectory to create products of high added value for the customer, the company, and the actors involved.

1.3 Research contribution

This thesis seeks to understand the organizational conditions that define the context of the decision-making process in chemical product design. It proposes an organizational framework to apply the existing chemical product design methodologies. The general objective of this research is:

To propose a methodology for the design of formulated chemical products within a company context.

The specific objectives of the project are:

- *Objective 1: To design a method for modeling the system of the product design process in cosmetic companies.*
- *Objective 2: To integrate and analyze stakeholders' needs into the proposed system model.*
- *Objective 3: To integrate a methodology for the design of cosmetic products in the defined system model.*
- *Objective 4: To validate the methodology by modeling a design system in a company (case study) of the cosmetic sector.*

Figure 1-3 shows the general research methodology implemented in this work. It starts with the Phase 1: the theoretical framework that demonstrates that researchers are increasingly interested in proposing methodologies to design new chemical products more successfully, but they almost never consider the organizational context in all its extend (Rivera Gil et al., 2022). Based on the literature review the objectives presented in this chapter were stablished. Phase 2 of the research methodology uses a system analysis to understand the design problem context, the actors, the processes, and their relationships in an organizational environment when designing chemical products. This is done through the analysis of several interviews with product formulation experts. Phase 3 established a strategy to integrate recommendations for the improvement of the design process to better respond to the needs of chemical companies and their organizational culture. Based on the results of phase 2 and 3, the design system and the recommendations responding to the needs of the organization, phase 4 shows a novel chemical product design tool that integrates organizational considerations to support design decisions. The document also contains the application of this methodology to a case study, which allows to test and to obtain feedbacks of the proposal.

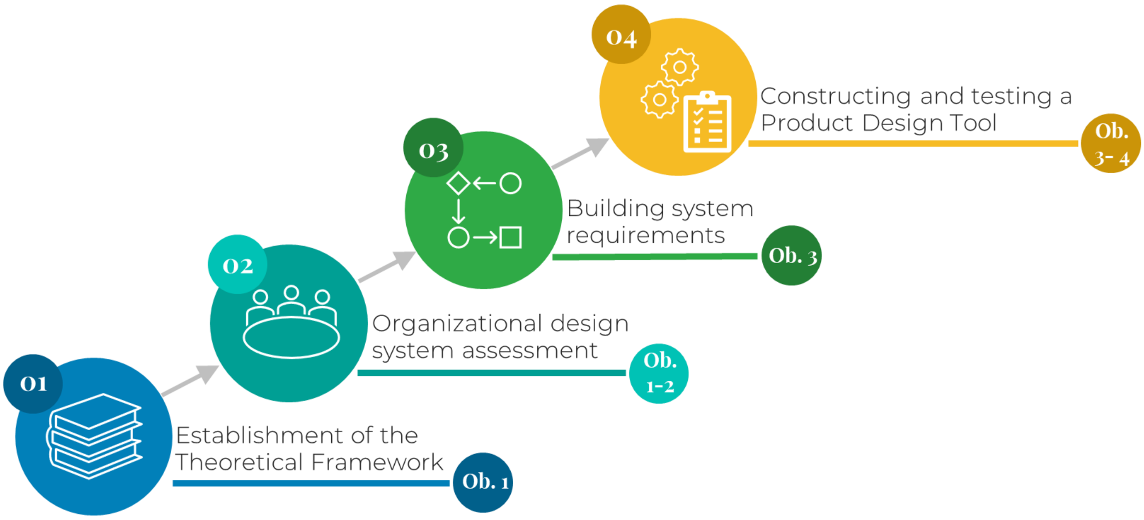

Figure 1-3 Outline of the research methodology applied to the research challenges related to specific objectives.

The general structure of the document is presented in Figure 1-4. The document is divided in seven chapters. The Chapter 1 introduces and presents the scientific positioning of the research. Chapter 2 presents the establishment of the theoretical framework based on a literature review. From this literature review, a vision of the influence of the design context on the design process is given. Chapter 3 presents a generic approach to map the activities, actors, information and resources of a design process of a specific company context. Chapter 4 presents the construction of a knowledge base used for the development of our tool to assist the chemical product design process. Chapter 5 shows the creation of the tool to assess a company's design process and to propose design improvement recommendations adapted to the organization. The application of the tool through a case study within a company is presented in Chapter 6. Finally, Chapter 7 presents the general conclusions of this work, as well as the perspectives and work to come.

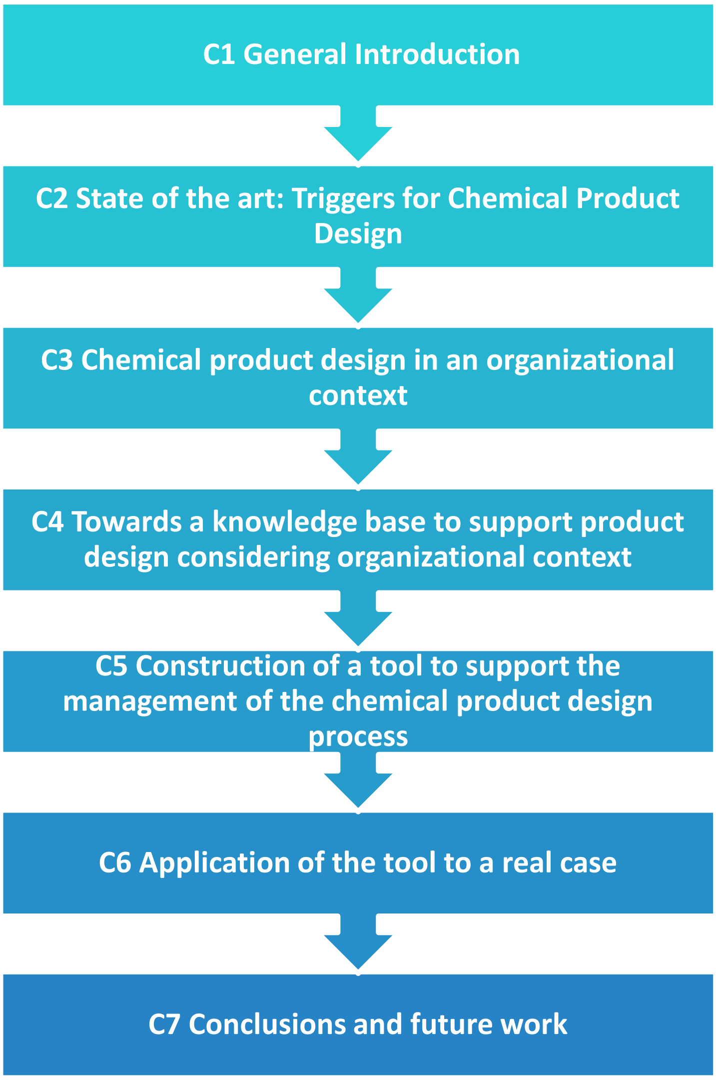

Figure 1-4 Structure of the document

2 State of the art: Triggers for Chemical Product Design

In this chapter, the current research problems associated to the chemical product design are identified. To do it, a systematic analysis of the scientific literature that proposes methodologies for chemical product design was conducted. The results of that systematic literature review containing the state of the art of the research, as well as the perspectives and conclusions, were published in the article “Triggers for chemical product design: A systematic literature review” in 2022 in the AIChE Journal (Rivera Gil et al., 2022)

2.1 Background in chemical product design

A product design project is a complex challenge, especially for the organization in which it takes place. It must simultaneously satisfy objectives and constraints, as well as meet the sustainability considerations that are highly relevant and specialized when dealing with chemical products. Additionally, it must meet the needs of stakeholders outside the company who participate directly or indirectly in the decision-making process. The outcome of the design process, the product, should help the organization to achieve its strategic objectives.

In general, the output of the traditional chemical design process is either the complete design of industrial production plants, the design of physical and chemical transformation processes, and perhaps, and less often, the specific design of chemical products. Each of these design processes must satisfy, in a sustainable way, the design requirements, which may come from the stakeholders involved in the design projects (Narvaez, 2014).

When designing a production plant, engineers deliver a collection of diagrams, drawings, specifications, lists, and data sheets aimed to mobilize resources for, acquisitions, construction, commissioning, and operation of the plant (Ullmann, 2005). Meanwhile, chemical process design has the objective of 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 final products (Narvaez Rincon, 2014). Plant and process design are well-known activities 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 (Hill, 2009). The latter should define the set of chemical compounds, the composition, and a physical structure for the product which can be materialized in molecules, mixtures, formulations, or devices(Cussler & Moggridge, 2011).

Various strategies and approaches have been created to assist chemical engineers in solving design challenges. The most prominent among them are tools that employ today's computing power as well as the benefits of simulation to offer product alternatives without incurring significant investments of resources. Even though there are several computer-aided methods and tools suitable for chemical-based product design (Suárez Palacios et al., 2020) , most of these have not yet been adapted to solve practical industrial problems (L. Zhang et al., 2020). These strategies and methodologies must, in addition, respond to a great diversity of chemical products in different industrial sectors, each with its own particularities. One of the main concerns of this study is to identify whether there is a generic chemical design methodology suitable for all types of chemical products and, if there is not, to determine the applicability conditions and limitations of the existing ones.

Among the variety of chemical products, it is important to highlight the differences between each one of them because they determine the design process. Cussler and Moggridge (2011) 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 integration (L. Y. Ng et al., 2015). 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 engineering (Ho et al., 2020). 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) methods (Austin, Sahinidis, et al., 2016; Bardow et al., 2010; Chemmangattuvalappil & Eden, 2013) 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.

Table 2-1. Chemical product types in different classification systems

Classification criteria of chemical products	**Chemical nature/micro-structure**			**Product complexity**	**Application**
Author	*(Cussler & Moggridge, 2011)	(Gani & Ng, 2015)	(Kontogeorgis et al., 2019)	(Smith & Ierapepritou, 2010)	(L. Zhang et al., 2020)
Categories of chemical products	**Commodities**	Molecules and blends	Devices	Basic/ functional chemicals	Coatings and sensors
					Process fluids
					Fertilizers and pesticides
	Molecules				Food
		Devices and functional products	Molecules	Structured products	Healthcare
					Skin protection
	Devices				Dyes and pigments
					Fragrances
		Formulated products	Structures	Configured consumer products	Special separations
	Structures				Energy provider
					Reaction promotion
					Functional device

Table 2-1 summarizes different ways to categorize chemical products presented by different authors and based on criteria such as product complexity, chemical nature, application field, among others. All the classification systems presented are complementary, and other classifications are possible. For the development of the literature review, the classification system proposed by Cussler and Moggridge (2011) 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 al (2020a) this kind of product is addressed as part of the largest set of formulated products; elsewhere they are listed in the classification of chemical specialties (Li et al., 2009).

2.2 Systematic Literature Review

This review included an analysis of 262 research papers and 336 patents, extracted from Scopus® and WIPO databases published between 1995 and 2020. These papers were classified according to the following criteria:

- Type of chemical product,
- Stages of the design process considered
- And whether for each research the organizational context was relevant.

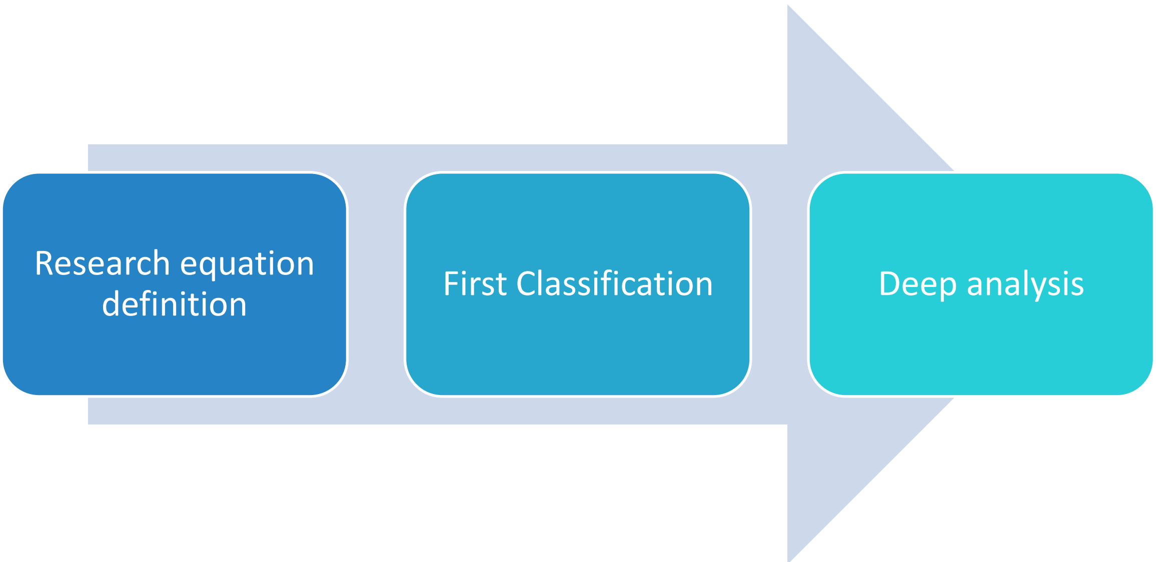

Figure 2-1. Approach for bibliometric analysis

The approach used for developing the bibliometric analysis is presented in Figure 2-1. It comprises three phases: research equation definition, first classification, and deep analysis. The approach was applied for two types of documents: scientific publications in chemical product design and patents related to cosmetic products.

In the research equation definition phase, a scanning of keywords was done using the Scopus search engine. The keywords and their combinations with results more adapted to our scope were used to compose the research question. The search equation comprises the keywords “chemical products design” and “methodologies” or similar in all search fields, as presented in Equation 2-1. 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 2-1. Bibliometric search equation

$$\begin{pmatrix} "chemi^{*}\ product^{*}\ develop^{*}" \\ OR \\ "chemi^{*}\ product^{*}\ design" \end{pmatrix} AND \begin{pmatrix} method^{*} \\ OR \\ approach \\ OR \\ decision\ making \end{pmatrix}$$

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 stages considered in the methodology (needs analysis, needs translation, alternatives proposition, selection, and process design), and if there is an organizational approach (it was identified if elements of the business strategy or activities conducted by an organization 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 they 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 2-2 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 2-2 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. This analysis is presented later.

After eliminating duplicated and unavailable publications, 658 journal articles were chosen for further analysis. Subsequently, these papers were graded as high, medium, or low in terms of their relevance to this study. Figure 2-2. shows that 257 documents were classified as extremely important.

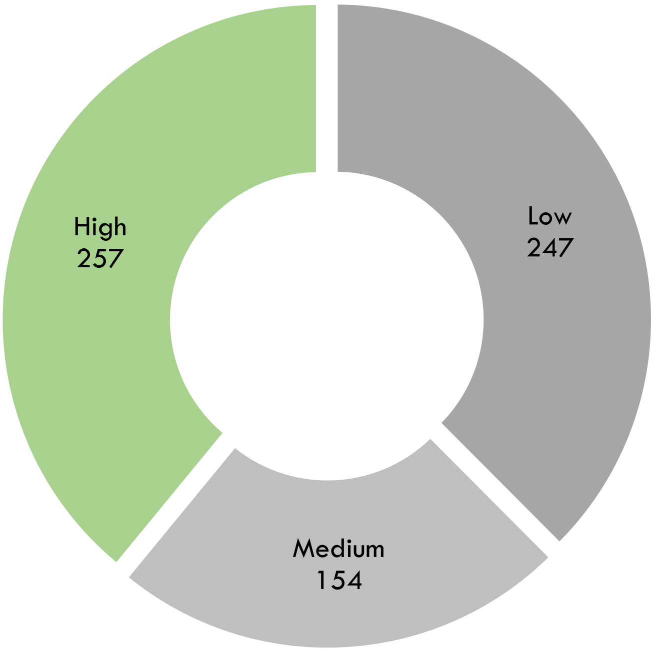

Figure 2-2. Results of the first classification of documents in scientific journals according to relevance to the subject

Only the most relevant documents (257) obtained after the deep analysis were examined. AppendixAppendix A provides a sample of those articles that also contain the product type "Formulated products" (it comprises 126 publications). There, the detailed evaluation of each document using the three classification criteria (product type, design stage, organizational context) is shown.

Figure 2-3 illustrates the rise in the number of scientific journal articles in the category of high relevance. Approximately half of the studies were published in the previous six years, indicating a recent and rising interest in researching chemical design approaches, notably those articles applicable to integrated and multiscale product design.

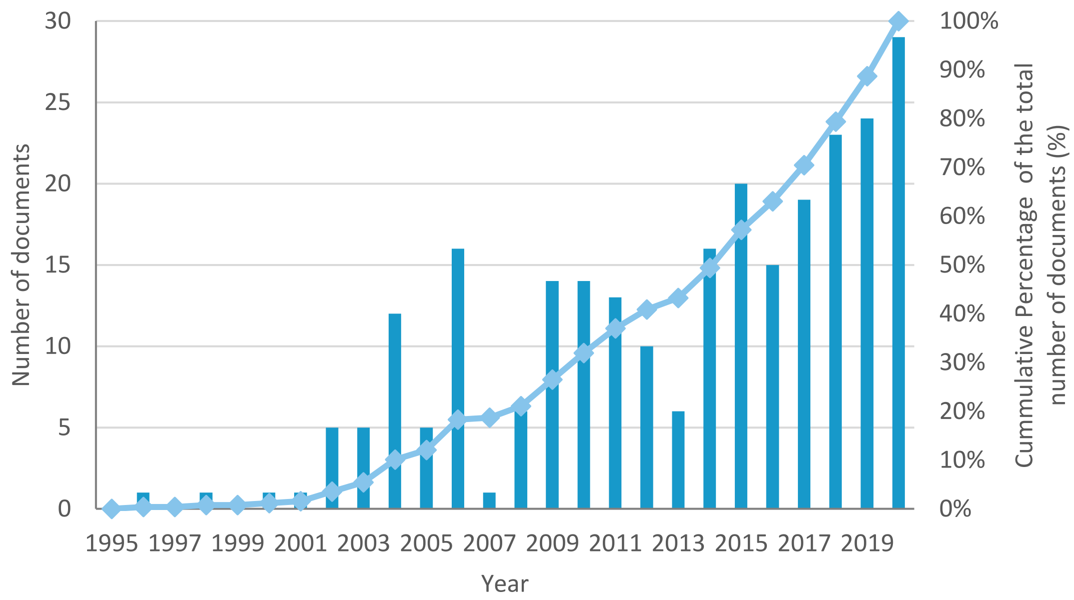

Figure 2-3 Evolution of publications in scientific journals concerning chemical product design methods for highly relevant documents. (Highly relevant documents, Accumulated percentage of highly relevant documents)

The high academic interest in producing publications covering the subject reflects an industry need and an interesting perspective on understanding which scientific developments are most relevant for application in product design organizations.

2.2.1 Product types

According to the analysis, 206 of the 257 documents in the high relevance category can be classified according to product types. The remaining 51 papers do not consider a specific type of product but rather they address issues such as general reviews and state-of-the-art studies, as well as pieces from industrial and academic viewpoints. Figure 2-4 shows the categorization based on chemical product types (commodities, molecules, devices, formulations). 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%).

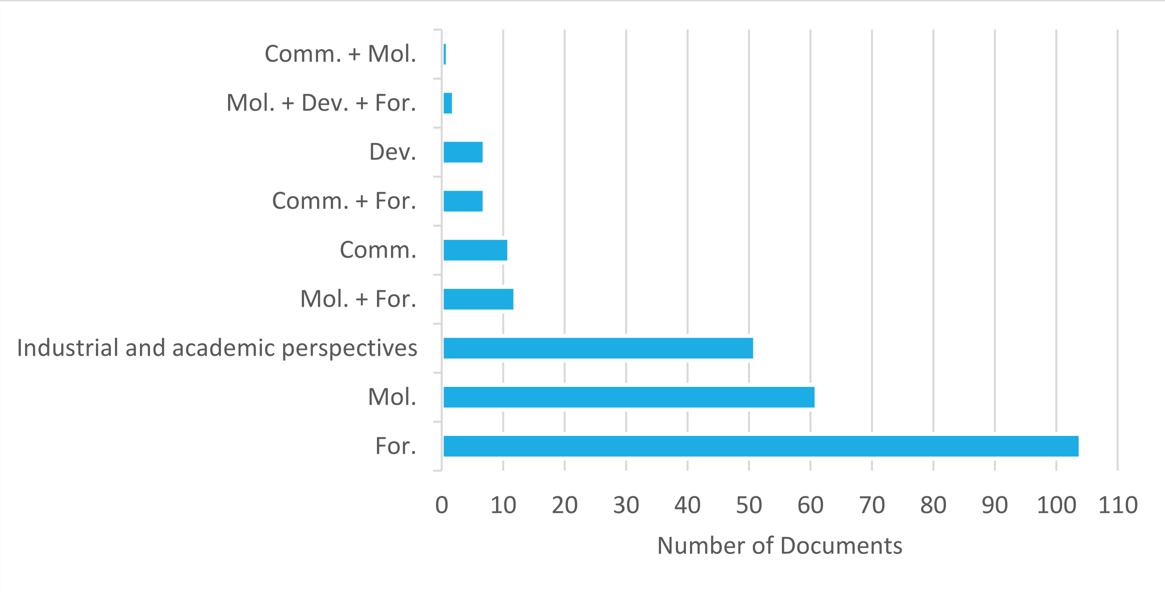

Figure 2-4 Classification of the documents retrieved from the bibliographic analysis and classified as highly relevant by type of chemical product mentioned in the methodology. From 1995 to 2020. (Comm. = commodities, Mol. = molecules, Dev. = devices, For. = formulated)

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 (Alshehri et al., 2020; Cardona Jaramillo et al., 2020; König et al., 2020; Xiang Zhang et al., 2019). 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 (Y. C. Chan et al., 2018; Derkyi et al., 2018; Smith & Ierapepritou, 2009).

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 models (Gertig et al., 2020). CAMD tools are widely used for the design of different applications, such as solvents (Chang et al., 2018; Rodriguez-Donis et al., 2018), pharmaceuticals (Houssein et al., 2020), among others. In relation to those documents considering two or more types of products, a general interest for integrated methodologies is presented. An example of these is the grand model for chemical product design (Fung et al., 2016), which develops a framework containing methods, tools, databases, and procedures for the design of molecules, formulated products, devices, and functional products.

Figure 2-5 presents the total number of documents of each product category (including mentions of papers that relate to more than one product type): formulations (126), molecules (78), commodities (19), and devices (9). It is worth mentioning that, as some writers have noted, there is a significant interest in formulated products for the proposition of product design methodologies in chemical engineering (Arrieta-Escobar et al., 2020; Uhlemann et al., 2019).

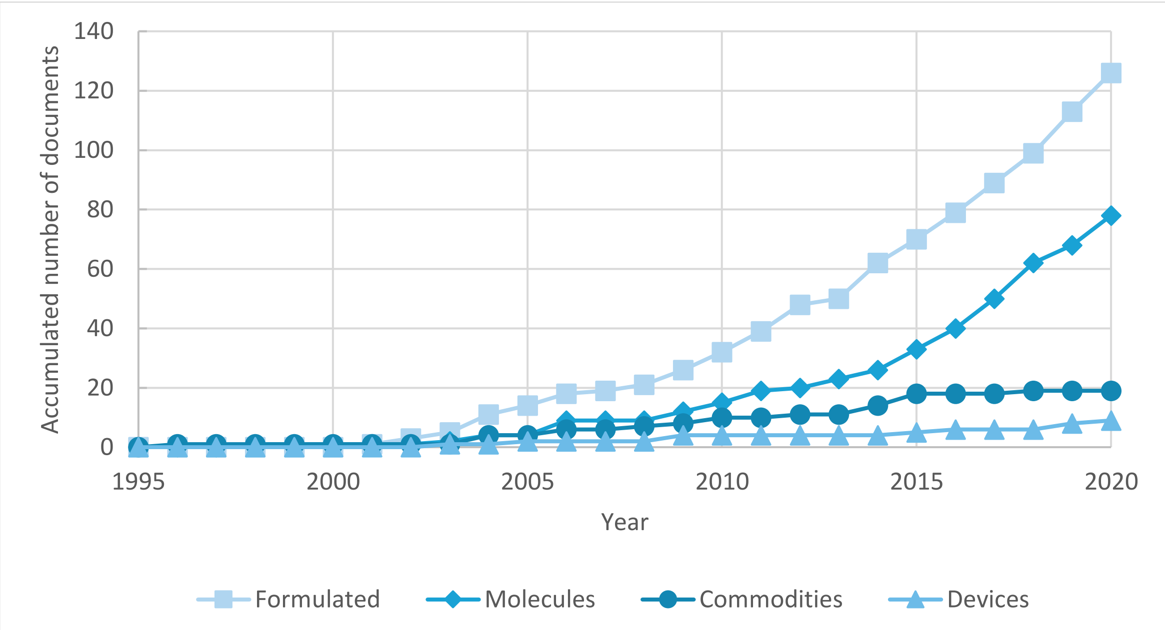

Figure 2-5 Accumulated product mention per year in scientific journals

The fact that formulated products have been leading the production of scientific material is again highlighted as a result of the transformation in the chemical industry, the attractive added value, and the interest of consumers. Challenges that will be faced by organizations in these industries

2.2.2 Design stages

Figure 2-6 shows the publications grouped according to the design stages mentioned in each publication. The most frequently studied are those that combines the “alternatives proposition” and “alternatives selection” phases. This group includes 94

(44%) of the total. In this group, most product design methodologies have an approach focused on solving the design problem by proposing a series of possible alternatives, and then, evaluating them according to their response to mostly technical design requirements. For example, in the work presented by Jonuzaj et al. (2016) a CAMD framework was applied in parallel with an optimization strategy; that framework enabled the proposition and selection of the best options according to target properties.

The second most repeated combination is the group of works 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 customer needs become an important constraint for the design (Y. C. Chan et al., 2018; Derkyi et al., 2018; Smith & Ierapepritou, 2009).

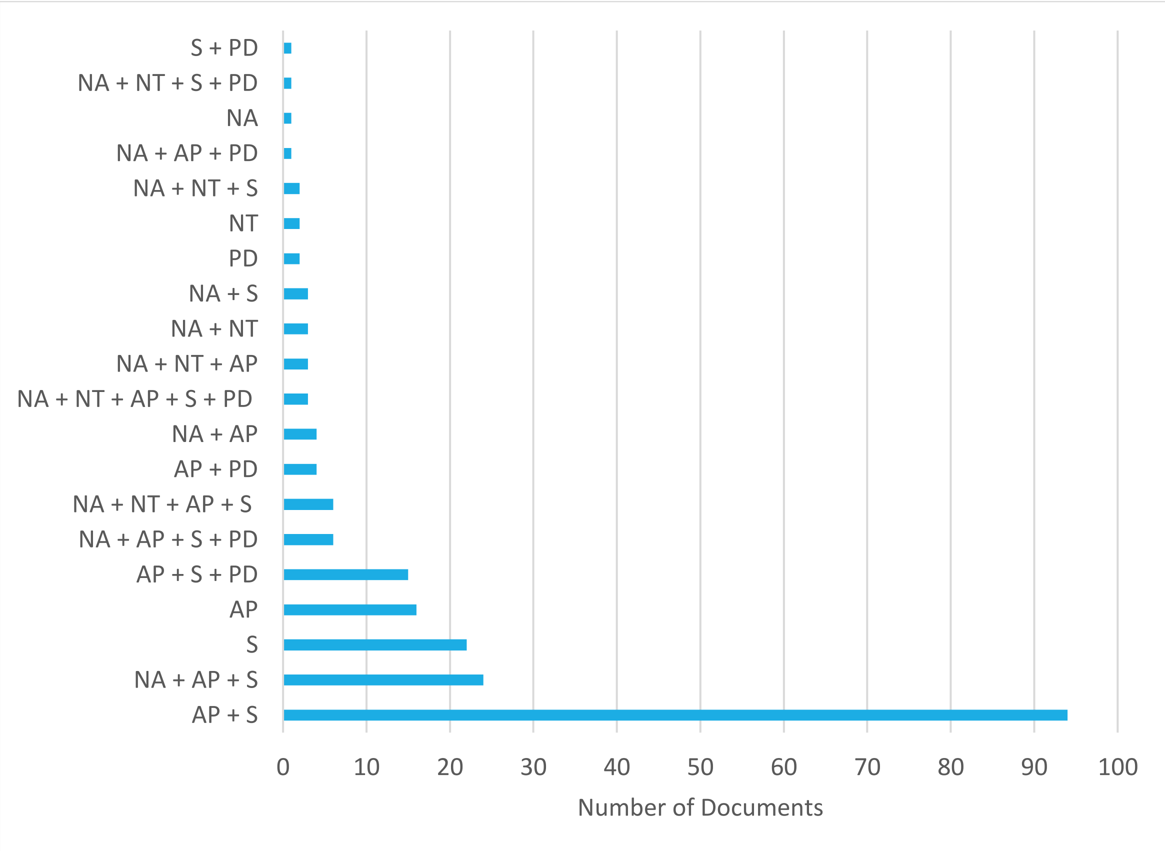

Figure 2-6. Classification of scientific journal documents by design stages (NA = needs analysis, NT = needs translation, AP = alternatives proposition, S = selection, PD = process design)

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 products (König et al., 2020). In total, there are 34 mentions of the “process design” phase within the reviewed articles. This is relatively low compared to the phases of “alternatives proposition” (178 mentions) and “alternatives selection” (179 mentions).

Regarding the phases of “needs analysis” and “needs translation”, the review found 58 mentions of the first and 20 of the second, which is not sufficiently considering that most formulated products are consumer products.

Therefore, it is perceived that the methodologies or tools found in the scientific papers lack a holistic approach where the context of product design and development is integrated.

2.3 Business strategy as driver for product design

Figure 2-7 shows the articles classified by product type and organization approach. Articles containing an organization 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. Figure 2-7 also presents the publications that in addition to the business approach also consider the business strategy of the company, i.e., the value proposition is reflected in the design process. According to the results, 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 integrating a business approach consider financial related variables (Yuen Shan Cheng et al., 2016) or marketing aspects (Yuen S. Cheng et al., 2009). Likewise, as highlighted in Figure 2-7, the methodologies for formulated products dedicate greater attention to the “business context” in comparison to other product types. Design methodologies that integrate business elements into their decision-making process seem to present holistic visions. They embrace additional dimensions such as supply chains (M. J. Bagajewicz, 2007) and government policies (Xiang Zhang et al., 2018). In the publications where the design methodologies also integrate the business strategy (12 articles), the notion of an internal organizational structure appears, and it is presented as a key notion for the design process. In those publications, operational, tactical, and strategic decisions are clearly distinguished (Fung et al., 2016; Heintz, Belaud, & Gerbaud, 2014; Marques et al., 2020).

Publications that mention formulated products were further classified by industrial sector, as shown in Figure 2-8. Most of the products mentioned (50 articles out of 126) correspond to the business to business (B2B) market, such as paints (Rafeqah et al., 2019) or inks (Chong, Eljack, et al., 2016). Generally, for that kind of products, specifications are well defined in technical terms. Second-ranked products are cosmetics, with 25 publications out of 126. The methodologies concerning this industry pose a major challenge because they must take into account that product properties should respond to customer needs (Smith & Ierapepritou, 2009). Additionally, regulations are more stringent in those industry domains.

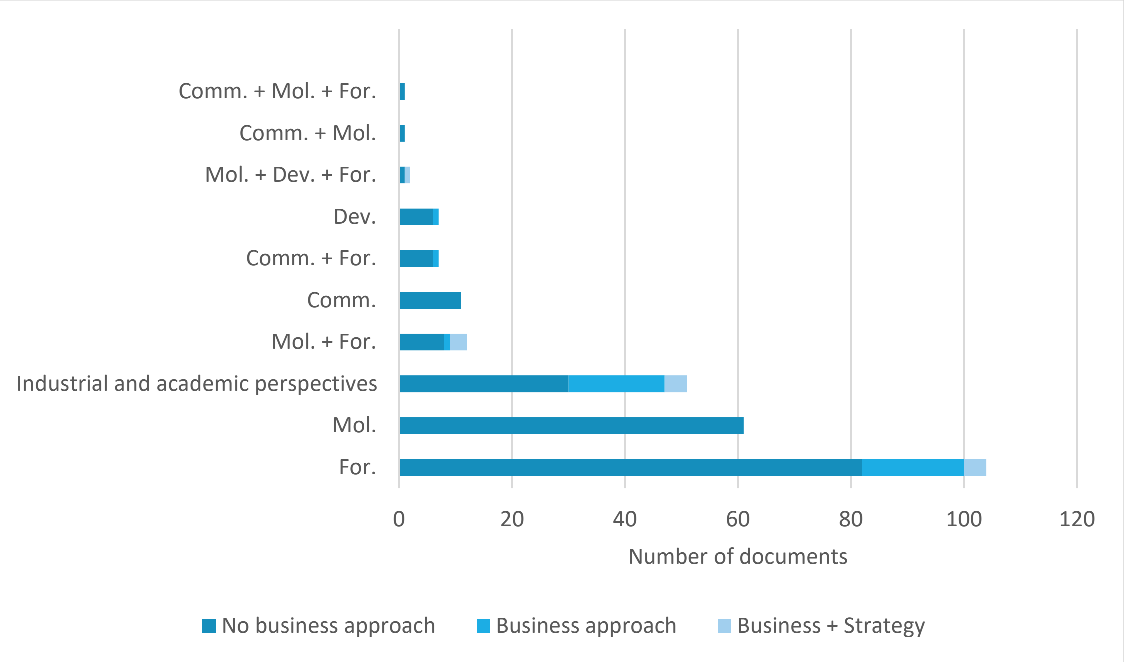

Figure 2-7 Classification of scientific journal documents by enterprise approach according to product type (Comm. = commodities, Mol. = molecules, Dev. = devices, For. = formulated)

The information presented up to this point has some clear findings that are the basis for the development of the present work. First, there is a strong tendency from the academic community for the thematic of chemical product design methodologies. Secondly, there is a profound change in the interest of chemical industry, from the B2B products towards specialized products and business to consumer (B2C) products. Additionally, there are not many methodologies considering how the company develops its design projects, how it is organized, and how information is shared between design actors. Finally, needs analysis in the design of consumer products are by far the most influential factor determining its success, but it is not the most studied one.

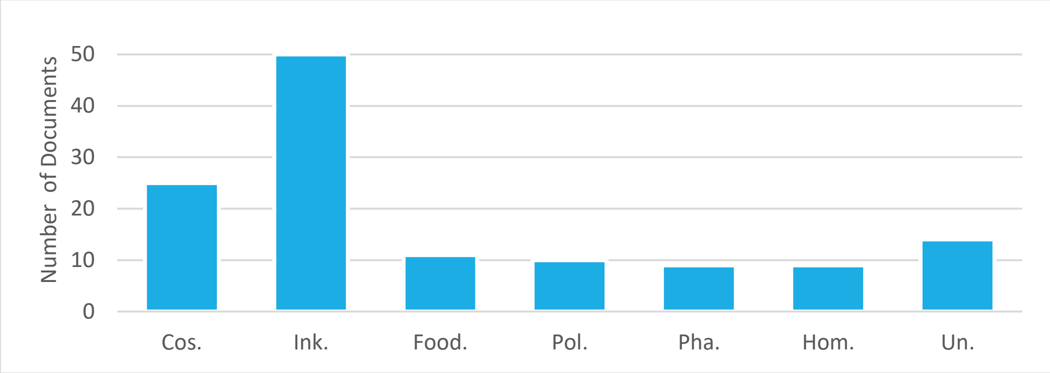

Figure 2-8 Formulated products classified by industrial application for the scientific journal documents (Cos. = cosmetics, Pha. = pharmaceuticals, Pol. = polymers and materials, Food. = food industry, Hom. = homecare, Ink. = solvents-fluids-paints-inks, Un. = unspecified)

2.4 Product design from an intellectual property point of view

As intellectual property becomes an increasingly vital part of doing business, and as the number of patent applications filed every year continues to increase rapidly, it is important for businesses of all sizes to be aware of the various aspects of the patent process. A single patent can provide businesses with a valuable competitive advantage in the marketplace, and an effective patent strategy can be key to a company's success (Brem et al., 2016). As part of our literature review, we included documents protected by intellectual property rights related to chemical products.

Given the nature of the patents, the analysis procedure could not be carried out in the same way as for scientific journal articles, so for this reason it was used the Equation 2-2. Figure 2-9 shows the four categories identified in the analysis of patents: new product; new process; packaging or applicators; and product customization.

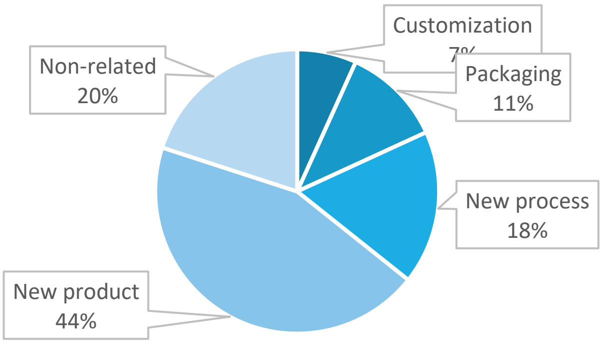

Figure 2-9 Percentage of documents in patent form by category

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 academic community. Interestingly, there are several patents in packaging (11%). Packaging design is an aspect that has been is completely disregarded in the reviewed articles, 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 work with a direct application in the industrial context.

Figure 2-9 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, a number of patents correspond to a methodology for the product individualization of Shiseido (Ando, 2020), 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 of the user.

Despite the evidence previously discussed in the review of academic papers, research on product design methods do not seem to be reflected in the industrial property documents protected by author's rights, however, it is highlighted that industrial efforts do not attempt to protect their new product design processes (in other words their design methodologies), but the products resulting from them (T. H. Chan et al., 2018).

2.5 From the state of the art to the research challenges

Based on the bibliometric review presented in subsections 2.2 to 2.4, it is possible to identify the research directions explored until now within the field of Chemical Product Design. It was found that formulated products were the most studied, accounting 46% of publications. Most of the publications (37%) were focused on the design stages of alternatives proposition and selection, while only 10% of them considered the phases of needs analysis and their translation to specifications. The consideration of an organizational context has not been widely explored in the design methodologies; only 17% of the documents assessed consider this aspect.

Figure 2-5 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). 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-scales (Kind, 1999), the production process is defined at the meso- and macro-scales (Costa et al., 2006), and product interactions with the users, the company, other stakeholders, and the environment occur at the mega-scale (Cisternas, 2006). 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.

The previous analysis allowed us to establish some key factors for the elaboration and implementation of methodologies for the design of chemical products that have not been considered in depth to date: the design context and the needs of the parties involved.

The role of the organizational context for product design should be considered for proposing future design methodologies, the design context is defined as follows: the political, economical, sociological, or technological environmental factors of the organizations. Companies designing formulated products must face a complex process that includes multiple individual and collective tasks. Design tasks done in interdisciplinary teams combining multiple capabilities and collaborating in order to achieve the design objective (Wang et al., 2021). All operational decisions made by the design team, such as the selection of ingredients, the definition of the manufacturing process, packaging design and brand definition, among others, have a direct impact on the other activities of the company and are reflected in the creation of value for the company itself and for other stakeholders (Kerm et al., 2012). Symmetrically, the evolution of the other activities within the company have an impact on design task. One example is the investment in an equipment with a higher performance rate or the strategic integration of a supplier. Therefore, chemical product design must be addressed considering both: the technical aspects, and the company context (the strategic objectives of the company, its resources, the needs of customers and the interests of those outside the company who may be involved (Cooper, 2019)). It is clear then, that design projects must be adjusted to the company's resources, strategy and business model.

2.6 Perspectives: from integrated methodologies and organizational context to formulation

According to the bibliometric 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. Among others, there are design methodologies that include financial and marketing models in global product design approaches such as those proposed by (K. M. Ng, 2004) and (Xiang Zhang et al., 2018). 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 problems (L. Zhang et al., 2020). This is similar in the case of the consideration of user needs in the design methodologies: only 22% of them consider the phases of customer need analysis and 8% of them the phase of customer needs translation. Despite of the little attention, the concept of the product and many decisions affecting the result are made during these two stages.

In relation to the aspects of organizational 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 stages proposed by Cussler (Cussler & Moggridge, 2011), only a small portion of these methodologies consider that organizational strategy influences the decision-making process. On the one hand, works that include hierarchical methodologies for companies' decision-making in regard to the design of formulated chemical products were found (Heintz, Belaud, & Gerbaud, 2014;

Lai et al., 2019). On the other hand, multiple studies summarize their approaches to company decision-making based on a product cost function (Y. C. Chan et al., 2018; Yuen Shan Cheng et al., 2016). 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 strategies. And, at an even higher level, other aspects, such as the supply chain (Taifouris et al., 2020b) and government polices (Xiang Zhang et al., 2018), which are useful as facilitators and/or constraints in the early stages of product design, should also be considered. In addition, chemical product designers must also be trained to develop interdisciplinary and business skills to allow them to be more context-aware, flexible, and creative to meet today's product design challenges. The study performed identifies the need to propose a holistic product design methodology from the early design stages, covering the assessment of customer needs and requirements of other stakeholders, as well as the business context where the design process is carried out.

2.7 Chapter conclusions

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 stages 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 stages that the analyzed methodologies entail, there is significant demand for the development of 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.

Thanks to the previous approaches this research will work on understanding the product design problem in two complementary axes:

- The technical challenges of the formulated products, i.e. the large solution space given by the combination of ingredients and the synergy of these with the manufacturing process.
- The organizational challenges given by the environment that the organization confers to the design activity.

This analysis shows the relevance of our general problematic: *"How to design formulated chemical products considering the company context in the design process?*

Figure 2-10 represents the context in which the chemical product design activity is carried out, showing the two key dimensions discussed earlier in this chapter, as well as the relationship with the inventive laboratories involved.

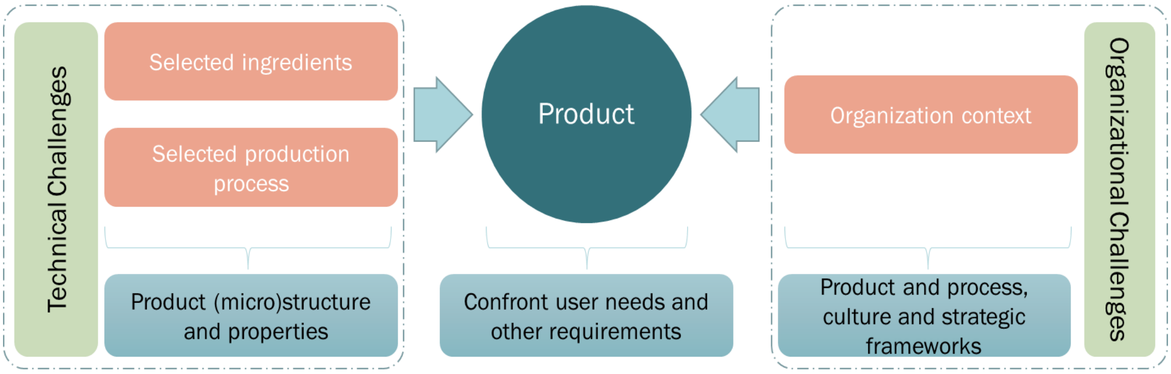

Figure 2-10. Chemical product design in a nutshell.

3 Chemical product design in an organizational context

This chapter seeks to analyze the design process regarding to its organizational context. For that, the design process is understood as a temporal system that appears when an organization initiates a design project. This system it is composed of actors, their activities, the product evolution during the conceptual development and the interrelations between all these elements. For the modeling of the system, in this research a characterization method is proposed. It is called the System Characterization Method (SCM). It is also applied in the analysis of eleven case studies: eleven design processes in eleven companies of the chemical sector (most of them corresponding to cosmetic companies). According to the SCM, the overview of the different design processes is based on information gathered through interviews with design experts involved in the analyzed design processes. This gives a realistic/experiential perspective on each company design process and allows for a better understanding of the company context and its effects in the design product.

Based on the analysis of the eleven cases, similarities and differences between the different design processes were identified, also the common practices and problems in companies and design teams. Additionally, the information and conclusions from this analysis are used later as the building blocks of the support design tool proposed in this research.

The results presented in this chapter were previously published in the 2021 conference paper "Towards a systemic approach for cosmetics formulation within companies: modeling the design system" in the International Association for Management of Technology Conference, IAMOT 2021(Rivera-Gil et al., 2021).

3.1 Conceptual framework: system analysis

Product design can be described in different ways regarding specific points of view. The technical perspective (i.e.: the understanding of the formulations developed by designers (Serna et al., 2021)), and the strategic standpoint (the perspectives of the company (Morel et al., 2013)). These are complementary visions of the design process, and are part of the decisional process that define the product and determine, in long term, the success of the product when it is launched to the market. Given the dynamic context and the multi-actor process of the decision making chain for product design, system modeling is a fundamental tool for understanding and capturing the complexity of the design problem (Salim et al., 2020). Consider the design process and the participation of the actors as part of the system provides a better understanding of the design problem beyond the technical aspects, adding a complement to purely academic source (Voinov & Bousquet, 2010).

To understand the design process, this research adopts the definition of *system* presented by Bosschaert (2019):

"A system is a set of objects and relationships between individual components that operate together, exchanging such things as information, energy, materials, value and other resources".

The following is a list of the elements that constitute any system. The elements are adapted to this research and to the product design process in an organizational context.

Actor: The term is used to refer to a role in the system. These roles can be played by internal or external stakeholders, departments of the organization, entities, decision makers, and other individuals involved in the chemical product design process. It is relevant to identify their needs or requirements, as well as the stages of the process in which they can have any influence (Voinov & Bousquet, 2010).

Relationships: A business may be seen as a series of interactions between the actors who have an interest in the activities of the company. In this research, these activities correspond to the product design process stages. Understanding the business and its process requires to considerate how these interactions function and evolve over the design projects (Parmar et al., 2010).

Process: Those activities or tasks that are developed by different actors, require and consume resources and modify the state of an object (Dori & Shpitalni, 2005).

Objects: An object is a thing that can be described for a set of properties such as size, mass, color, material composition, geometry, etc. (Bosschaert, 2019). The product is an object that evolves during the design process from the first conceptualization until it is launched to the market. These four elements will be the basis of the model on which this research is based.

3.2 System Characterization Method

This research proposed a method for modeling the design process inside organizations called the System Characterization Method (SCM). The method applies a system analysis approach to characterize the design process and it is based on a previous research in system thinking (Bosschaert, 2019) and a system modeling method for product design (Chavy-Macdonald et al., 2019). Its novelty corresponds to the systemic analysis of the product design process, as an integrated activity, from the need analysis stage to the selection of ingredients and the design of the production process. The SCM aims to identify the actors involved in the design process, and subsequently, to analyze the relations between the actors and the information and material fluxes across the system. The goal of the method is to perform a system analysis of the design process of formulated chemical products. For this, the product design process is theorized as:

A temporal decision-making system that appears when a company decides to initiate a project to launch a new product.

The SCM analyzes the design process considering three key aspects to define the boundaries of the system:

- Nature of the product: In the chemical industry there is a multiplicity of products of different complexities and areas of application. This method focuses on formulated and consumer products such as some products in cosmetics, foods, and pharmaceuticals. Special interest is given to the analysis of cosmetic design processes.
- Activities of the company: The method focuses specifically on those organizational activities related to the design and development of products.

- Company context: As an important axis, the strategic and tactical contexts of the company are considered essential to the system analysis.

The application of the SCM comprises three stages as shown in Figure 3-1. The steps to apply the SCM are described following:

Figure 3-1 System characterization method (SCM) applied to chemical product design (Source: our research).

3.2.1 Data collection

The objective of this step is to capture data about the design process developed by a particular organization. For that, information regarding the phases of the design process, the actors involved, and the resources shared is collected. The SCM proposes to collect this information with semi-structured in-depth interviews with industrial experts involved in design projects (experts which are also decisional actors in the design process). Aiming this purpose, an interview protocol divided in three main parts is proposed as presented in Table 3-1:

Table 3-1 Interview protocol applied to chemical product design experts to perform the data collection phase of the System Characterization Method

	Objective of the phase of the interview
PART 1: Meeting the interviewee	·Determine the profile of the interviewee, experience, area of work, career, and position in the company.
	·Know the overall experience in formulated product design of the interviewee.
	·Describe the current company, size, how the company is organized, where the company operates, what is the company value proposition, as well as the mission and vision.
	·Identify the interviewee’s position in the product design process within the organization.

	Objective of the phase of the interview
	·Know if the interviewee has designed products within other organizations and which roles he played.
PART 2: How product design is carried out	·Know the formulated product design process in which the interviewee has participated.
	·Understand which the areas of the company are involved in the design processes and identify the relationships among these areas during the design process.
	·Understand the decision-making process within the design project how is the information gathered by different actors all along the design process and what is the perception of hierarchies inside the design teams.
	·Identify the information the interviewee uses to make decisions, and when it is required and shared.
	·Understand, according to the interviewee, the moments of the design project when collective decisions are required.
	·Understand what information allows the interviewee to make easy decisions, including when the different actors of the design team should be involved.
PART 3: Chemical engineering studies and product design	·Identify the relationship among the academic background of the interviewee and his/her performance in the product design activity.
	·Establish if the interviewee has identified areas for improvement in the professional training programs to develop better skills for product design tasks.

In addition, to the reach the objectives described in Table 3-1, the interview protocol asks the experts about the company context and its effects on the chemical product design, to gather information related to the strategy, target market, product quality, differentiation criteria respect to competitors, degree of product customization, perceptions linked to the products, use of installed technological, size and versatility of the production plant, channels of diffusion, and frequency of product renewal.

3.2.2 Data screening

In this step, the data collected on the step one is organized and represented with the structure of the matrix on Table 3-2. The representation allows the researcher to standardize and eventually to compare the information collected in the interviews with different types of experts in different types of companies. In the Table 3-2, the design process is divided into design stages (Ds). For each Ds a complete list of the actors is collected, and their functions are described. Comments regarding the organizational strategic frameworks influencing design projects are registered. Opinions on the shortcomings or positive aspects of design stages are also registered.

Table 3-2 Generic data screening matrix for the information collected in step 1 of the System Characterization Method

	Design stages	***Stage Objectives***	***Actors***	***Additional Comments***
Interviewee identification	Ds_1	Ds_1 Objective	$S_1, S_2 \ldots S_n$	Ds_1 Comments
	Ds_2	Ds_2 Objective	$S_1, S_2 \ldots S_n$	Ds_2 Comments
	…	…	…	…
	Ds_i	Ds_j Objective	$S_1, S_2 \ldots S_n$	Ds_j Comments

3.2.3 System characterization

The final step of the SCM, it is based on the information gathered from the interviews and organized in the form described previously, the key points of product design processes are identified and translate by the research team into the SCM scheme. The structuration of this points is based on the one hand, in the identification of the relationships between actors, as well as on the analysis of the design process, the activities developed and the resources consumption. On the other hand, significant remarks from the experts about the effects of the design context in the design process are highlighted. Figure 3-2 presents a general description of the analysis of the data collected with the experts, on the one hand looking for common points based on the design processes described during the interviews (later developed in chapter 4), and on the other hand to understand the observations, opinions, and thoughts of the interviewees to set the basis for a generic characterization of the context in which the chemical product design activity is carried out.

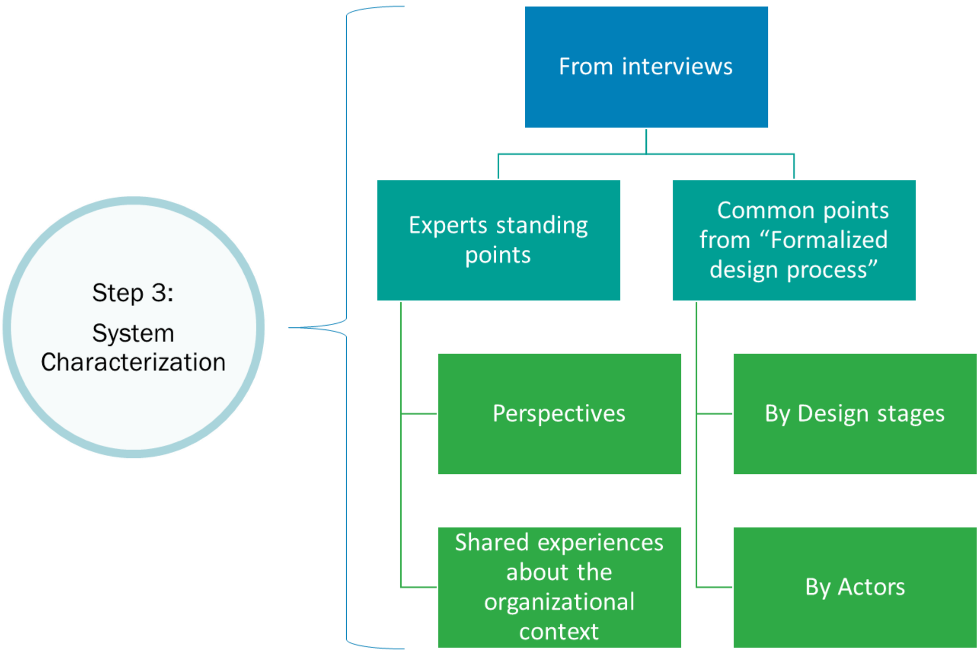

Figure 3-2 General structure for system characterization

3.3 Application of the SCM

Industry experts with extensive background in product design in the chemical sector were contacted for this study. A total of eleven experts, mostly chemical engineers, were interviewed using the protocol presented in Table 3-1 (most of them corresponding to cosmetic sector). All the interviews were carried out via Microsoft Teams during the second half of 2021. Each interview spends about one hour. Remarks about the general characteristics of the process and the corporative strategies of the companies were also collected.

The analysis of information gathered from experts with different backgrounds, in a variety of companies, allows us to recognize emergent properties and generalities and to characterize the system previously described (section 3.2) within the boundaries defined regarding the nature of the product, activities of the company and company context.

Table 3-3 summarizes the main characteristics of interviewees. As presented in the protocol, Table 3-1. The conversation focused on their professional experience, the chemical product design process, and their views on the education of chemical engineers and the product design activity. The experts were selected considering that they have worked at all levels of the organization to face the problem of product design; strategic, tactical, and operational levels. This transversality of the experts permits to have a general vision of the design process from which is possible to understand the challenges faced by the design teams.

Table 3-3 Profile of the experts interviewed for SCM application

	Profile	Time of experience	Role	Type of company	Industry
1	Chemical engineer	6 years	Formulator	Latin American multinational	Cosmetic
2	Chemical engineer	5 years	Formulator	Latin American multinational	Cosmetic
3	Chemical engineer	4 Years	Supplier	National SME	Cosmetic
4	Chemical engineer	3 years	Owner Formulator	National SME	Cosmetic
5	Chemical engineer	2 years	Owner Formulator	National SME	Food
6	Chemical engineer	11 Years	Formulator	Multinational	Pharmaceuticals
7	Chemical engineer	5 years	Owner Formulator	National SME	Brewing/Food
8	Chemical engineer	10 Years	Formulator	Latin American multinational Multinational	Cosmetic
9	Chemical engineer	15 Years	Formulator	National Latin American multinational Multinational	Cosmetic
10	Pharmaceutical chemist	20 Years	Formulator Researcher Columnist	Latin American multinational	Cosmetic
11	Chemical engineer	16 Years	Formulator Director	Latin American multinational	Cosmetic

3.4 Results of the application of SCM

3.4.1 Data collection

According to Table 3-3, the panel of companies represented by the experts also provides a diverse picture of the formulated products industry, although most of the experts belong to companies working in the cosmetics industry. There are also companies from other formulated products industries such as pharmaceuticals, food, and brewing. Regarding the type of the companies the interviewees work with, seven are multinationals, most of them with focus on Latin America. In addition, four experts are representatives of small and medium-sized companies (SME) with national presence (Colombia).

Regarding the role played by the experts, most of the interviewees identify themselves as “formulator”. Also there is presence of companies of entrepreneurships in formulated products-based, as well as experts whit a researcher background. The role of “formulator” refers to a broader term in the case of the interviewees. It does not only refer to the technical aspect of define the components, composition, micro and macrostructure and production process of a chemical product. This role is played simultaneously with other roles inside the company, at different levels, including project managers, area managers, project leaders, project coordinators, etc.

3.4.2. Data screening in the analyzed companies

Experts were asked to describe the chemical product design processes they have worked in; the data collection and posterior analysis were performed using the steps of SCM described in this chapter. Table 3-4 presents a summary of the design processes shared by the experts, showing a list of the actors and design stages mentioned during the interviews.

Table 3-4 List of design stages and actors mentioned by experts

Expert	List of design stages	List of actors
1	Preliminary trend studies Brand needs Product conceptualization Technical feasibility Product technical concept Pre-prototype Technical validation Prototype User Validation Legal Validation Scaling-up Process standardization Project closure Accompaniment to production	Brand representative Consumer External consultant Formulation team Graphic and communications teams Legal team Logistics and packing team Marketing Product Manager Production plant team Regulatory entities Supplier Test Laboratory
2	Ideation Conceptualization Feasibility Formulation Scale transfer Prototype study Approval Technical approval Monitoring and reformulation	Brand representative Company directors Shareholders Consumer Formulator team Legal and regulatory equipment Packaging team Production plant representative Project manager Safety laboratory Supply chain team Test laboratories
3	Establish customer needs Positioning in the market Define formulation idea	Formulator Manager Marketing Department

Expert	List of design stages	List of actors
	Prototyping Technical development Legal consulting Establish supply chain In-plant production	Owner Research and development team Supplier
4	Market research Users need analysis Supply chain research Formulation screening Prototype tests Final feasibility Transition to production	External manufacturer Formulator Owner Supplier User
5	Benchmarking Define marketing strategy Technology development Prototype development User testing Reformulation Production Commercialization	Academic Partner Directives Producer associations Project incubators Research and development team Sales department Suppliers
6	Needs analysis Benchmarking Idea generation Innovation plan Initial formulation Packaging definition Production process definition Safety testing Efficacy testing Technical validation Definition of production requirements Regulatory review Sales plans Production Monitoring	CEO Commercial team External laboratories Legal team Marketing team Packaging team Production plant Project Manager Quality team Research and development team Users
7	Market research Idea generation Design of formulation experiments User testing Reformulation Expert testing Establishment of the supply chain Production Sales plan Sales	Formulator Industrial Ecosystem Manager Production Plant Sales Department Suppliers Users
8	Definition of marketing strategy Market research Feasibility of design proposal Project risk management Initial formulation Technical feasibility definition Prototype Laboratory testing Legal feasibility Supply chain assurance Sales campaign Production	Board of Directors Consumer Contractors Finance team Formulator Logistics team Marketing team Plant team Project Manager Purchasing team Regulatory entities Research and development team Sales team Suppliers
9	Consumer study Marketing plan Product ideation Concept validation Preformulation	Consumer Logistics team Marketing team Production team Project manager

Expert	List of design stages	List of actors
	Prototype validation Formulation Reformulation Legal validation Production plan Logistics and inventories Scaling Production	Regulatory bodies Research and development team Research and development team Sales team Suppliers Testing laboratories
10	Marketing plan Consumer needs analysis Conceptualization Formulation Prototyping User testing Risk analysis Negotiation with other departments Production plan Production	Consumer External consultants Finance team Formulator Marketing team Plant team Project Manager Research and development team Suppliers
11	Market trend study Needs analysis Conceptualization Formulation Prototype testing User testing Technical validation Pilot scale validation Industrial development Scale-up Production	Analytical laboratories Financial team Formulator Logistics and packaging Management Marketing team Production plant Regulatory team Research and development team

When analyzing the design stages of the different organizations, it can be seen that there is a difference between them in the number of stages formalized in the different processes; each company defines how to structure its own process (stages and actors) according to its capabilities, resources, experience, knowledge, among others. However, the same objective can be achieved with different process structures. Two of the eleven representations of the design process described by the experts are presented below (Examples 1 and 2). The objective with these examples is to show the differences of two companies in terms of organizational structure around the design process.

Example 1

Table 3-5 presents in detail the results of the application of the steps 1 and 2 of the SCM to one the companies represented by the expert #1. This company is a multinational company focused on the cosmetics market. It designs, produces, and sells products for personal care, skin care, hair care, perfumery, and makeup.

Table 3-5 System understanding - Design system information – company 1.

Design stages	Actors	Stage Objectives	Strategic and Additional Comments
Preliminary trend studies	• Brand representative • Marketing • External consultant • Consumer	Process of studying market trends	People who are responsible for the availability of raw materials and production process capabilities are not involved at all.
Brand needs	• Brand representative	Establish how the brand is going to act in the face of market trends	No Comments
Product conceptualization	• Brand representative • Marketing • Consumer	Establish product claims	No Comments
Technical feasibility	• Brand representative • Formulation team • Legal team • Production plant team • Logistics and packing team • Graphic and communications teams	Multi-stakeholder consultation	At this stage, all the design team can give their opinion and narrow down the product project to a viable concept.
Product technical concept	• Product Manager • Brand representative • Formulation team • Supplier • Logistics	Review of corporate attributes (philosophy, work ethics)	A key step is to set cost limits, establish relationships with suppliers. The possibility of acquiring new technologies or raw materials is also investigated.
Pre-prototype	• Formulation team • Supplier	Iterations to formulate a product according to the above requirements.	At this stage the decisions are made by the formulation team. When it is necessary to have the input of all the area leaders, the process becomes delayed.
Technical validation	• Test laboratory	Establish product safety and compliance with desired claims	No comments
Prototype	• Formulation team • Production plant team • Packaging team	Iterations to study package compatibility, feasibility in a pilot plant according to the formulation	No comments
User Validation	• Consumer • Test Laboratory • Brand representative	Safety and acceptability checks with volunteers	Usually, the brand decides if the results of the validations are sufficient to continue the process.
Legal Validation	• Formulation team • Legal team • Regulatory entities	Registration of the product and the process with	Formula elements can be adjusted to have a margin of error for the regulatory authorities.

Design stages	Actors	Stage Objectives	Strategic and Additional Comments
		regulatory authorities	
Scaling-up	• Formulation team • Production plant team • Logistics and packing • Team • Test Laboratory	Iterations in production plant to meet specifications	In many cases it is impossible to move to industrial production, it must be decided whether to cancel the project or return to the formulation stages.
Process standardization	• Formulation team • Production plant team • Regulatory entities	Adjust formula, the process of production, and update to regulatory authorities	The formulation team must ensure that the area executes the designed product as intended.
Project closure	• Product Manager	End of product design project	No comments
Accompaniment to production	• Formulation team • Production plant team	Verifications and accompaniment to the production phase once the product is on the market.	No comments

The design process (13 stages) in Table 3-5 involves multiple actors in each step (14 actors, ten of them internal to the company). The described process is developed thanks to a clearly defined structure by the organization, where the actors always play the same role and their activities are clear throughout the design project. This structure follows the guidelines established by the organization. A bureaucratic (given the complexity of the organization with multilayered systems and processes) and hierarchical structure (chain of command to respect) is also imposed on the organization, the design team is confronted with these constraints for certain decisions that are key in the design process. The actors of this organization are constantly engaged in diverse new product projects, so the company has organizational departments specialized in the different types of activities that are required in the design process; for example, the legal team comes to have an important influence on various aspects such as ingredient selection schedules, product claims and time to market.

Example 2

Table 3-6 shows the design process of a recently established company (less than five years), classified as a very small company (Ministerio de Comercio, n.d.). This company is focused on the production of cosmetics. It has a value proposition that does not focus on mass consumption, it is interested in niche markets, respectful of animal rights and the environment.

Table 3-6 System representation - Design system information – company 4

Design stages	Stakeholders	Stage Objectives	Additional Comments
Market research	• Owner • Formulator	Understand market trends with respect to the company's philosophy. first contact with competitors' products.	First contact is made with suppliers to see feasibility of inputs, limited resources at local disposal A trend analysis together with the company's vision/strategy is crucial for product design. Find allies in contract manufacturer, suppliers, and marketing.
Users need analysis	• User • Formulator • Owner	Understand the sensory expectations in terms of aroma, form, use, presentation, as well as the expected functionality.	Product proposals tailored to local consumers
Supply chain research	• Formulator • Supplier	Identify the availability of local raw materials for the candidate products, including primary and secondary packaging, in addition to the ingredients	No comments
Formulation screening	• Formulator	Initial basic formulations, to reject or approve formulation hypotheses	No comments
Prototype tests	• User • Formulator	Test the proposals that have been developed in the laboratory with users	Essential to generate rapid prototypes for testing with users, maintaining a basic formulation
Final feasibility	• Formulator • Owner	Establish technical, regulatory and value proposition satisfaction feasibility prior to a production contract.	The design process is evolutionary in parallel to the normative developments. To move to a final formulation, consider capacity, inputs, packaging, etc.
Transition to production	• External manufacturer • Formulator	Transfer the formulation to the manufacturer	Work with third parties in case of scaling up from production to plant; maintain quality controls.

In this case, the process has a less actors (five, and only two are internal to the organization) and the process has seven stages. The structure of this organization is not hierarchical nor bureaucratic. The design team has limited access to resources (human, technical, financial), therefore the experience and knowledge of the actors of the organization are very useful in the design process. In this enterprise, the formulator and managers directly engage users by confronting them with ideas, concepts, and prototypes to obtain rapid design feedback, these activities allow the design team to understand the needs and preferences of its user. Suppliers and producers become an important source of information in the company's process thanks to a close and dynamic relationship, where the design team can easily consult and ask for recommendations. Since the process is not formally structured, there is flexibility in the internal processes.

3.4.2 SCM approach analysis

The system analysis can be used to describe the design process in different organizations. In general, thanks to the description of the design processes it can considered that:

- Organizations adapt the design process (i.e. they define the actors involved, the organizational structure of the company's internal processes), strategic objectives of the project, and resources available for the design project (technological, financial, etc.), according to their circumstances and objectives. Therefore, although the design processes have the same objective: "to design and develop a product", are different from one company to another. In addition, according to experts, the design process is modified evolving from project to project within the same organization.
- In the opinion of experts, communication difficulties between stakeholders may arise when the design team finds itself in the context of an organization that is governed strictly by structured and hierarchical processes. According to them, this difficulty leads to a loss of clarity between the stakeholders involved in the project.
- According to the experts, the objectives of the design project are achieved in a context that has resources such as knowledge, raw materials access, equipment, and state-of-the-art processes, among others. It should be noted that knowledge, as part of the company's experience in this type of projects, is one of the fundamental resources to successfully complete the design project. This knowledge allows the design team to adequately address the projects even when resources are not enough. However, there does not seem to be a widely applied knowledge management system in the studied cases.

From the designer's point of view, the SCM can provide a global view of the design process, of the actors and decisions involved at different levels of the organization, and thus lead to a more informed decision-making process.

Moreover, from a research point of view, this analysis allows the design team, at a later stage, to propose design methodologies adapted to the design context (chapter 5), which in turn could allow the designers to achieve a better appropriation of the design process by the companies and actors involved.

In general, four key points stand out when comparing the design process of the eleven companies:

Heterogeneity: There is no single route for the design of cosmetic/formulated products, even the same company implements different routes for different product design projects. Each one is adapted to its own context and has specific characteristics according to the organization's resources.

Corporate governance: All design processes depend on the company's interests, strategy, internal processes, knowledge and resources. The outcome of any design process will reflect the organization's ability to articulate its tangible and intangible resources.

Active participation of stakeholders: Design decisions are not only made by internal stakeholders of the organization. Decision-making depends, as appropriate, on relationships with external stakeholders, notably consumers, and others such as suppliers and service providers.

3.5 Chapter conclusions

This chapter proposes a generic methodology to understand the temporary design system formed within a company during a design project. In that system, the design stages, the actors, and their information exchange process are represented. The information for the analysis of the system is collected through semi-structured interviews with members of the design teams. The method was applied to eleven companies. It generates systems with a clear view of the relationship between actors and their role in the design process. This formalization may enable the design team to better understand the context of the design process, and thus, make more informed design decisions. Moreover, it can be used as a management and communication tool between the design teams and the project managers.

Based on the analyzed companies, it is possible to realize that the actors and their relevance change as the design progresses. Moreover, the representation of the system allows the design team to know in advance the type of requirements they will face during design at early design stages, which may allow them, in the long term, to foresee requirements and avoid unnecessary redesign loops due to unexpected missing information.

The insights about the real design context of chemical product design are integrated in the development of the design methodology presented in this research. Considering the business context enable a global appropriation by the design team. Such a vision not only facilitates decision-making during design but also gives a clear view of the information flow from the early design stages. Additionally, it could enable innovations by affecting the product itself, the design process, the relationship between internal and/or external actors. Furthermore, the relationships between the actors, the design process, and the business context are dynamic, consequently, a complementary holistic approach is required.

4 Towards a knowledge base to support product design considering organizational context

The objective of this chapter is to develop a knowledge base for decision-making related to the design of formulated chemical products in organizations. This knowledge base is developed considering the information shared by interviewed experts (Chapter 3) and it is later used in Chapter 5 for the proposition of the methodology to assist the chemical product design process.

The knowledge based provides design heuristics, i.e., design recommendations which can be used by organizations to evaluate, understand, improve, or create their own design methodologies considering their context and resources. It was constructed by extracting key design information from the experts' interviews and by analyzing this information according to three types of criteria: phases of the design process, involved actors and the organizational context. The resulting knowledge base contents recommendations based on structured information of design processes that have led to the development of successful products. It is focused on design processes for cosmetic product companies.

4.1 Introduction to a knowledge base approach

The objective of a knowledge base is to facilitate the understanding of a topic and make knowledge accessible. Thus, it gives sense to information and enable better informed decision. A knowledge base in the domain of knowledge management, provides the means and documents that can be exploited by decision makers (Krishna, 1992) to, in this case, design products. Its construction faces several challenges: it should be adapted to the specific topic, in this case to the design process, which is done by multidisciplinary collaborative teams; it should organize heterogeneous information coming from diverse sources, as the involved in the design process; and it should be managed, updated and refined according to the advances in its field of application, maintaining coherence between new and old knowledge (Jasimuddin, 2006).

In general terms, knowledge can be classified into two categories. It can be explicit and implicit. The former is based on well-established facts while the latter is based on know-how, experience and intuition (Kimura et al., 2004). Explicit knowledge is available in documents, databases, and computer information systems. It is structured thus it is easy to share. Explicit knowledge is normally clear and accessible, and it is usually well recognized by the design team. An example of explicit knowledge in chemical product design corresponds to established physicochemical specifications, models, equations, formulas, and well-known production process fundamentals, among others.

On the other hand, the implicit knowledge is difficult to acquire, to transmit and to be conserved within the design teams. This knowledge is also highly related to the design context because it is the result of the trajectory of both the organization and the individuals. Implicit knowledge evolves with practices, change in organizational structures, design habits, and development experiences, among others. It remains implicit to individuals and is eventually lost if it is not codified, transferred and shared within the organizations (Kumar Mohajan, 2017).

It was previously stated that chemical product design can be understood as a system comprising the product in development and the organizational context where it is developed. In this case, knowledge is not only a structured information about the product but it is also information in context (Chandrasegaran et al., 2013). Considering the above, this chapter presents the construction of a knowledge base for chemical product design considering the organizational context that formalizes the implicit knowledge of several design experts from different chemical product design processes and organizations. The elicitation, analysis, and representation of this expert knowledge in a knowledge base, enables it exploitation by actors in organization for its application in chemical product.

4.2 Building method of the expert knowledge base

The knowledge base developed in this research comes from the information gathered through the interviews with experts presented in Chapter 3. Here, key information related to the design process in its context is extracted from the interviews and then it is analyzed according to a framework to give it a structure. Figure 4-1 shows the method used for the construction of the knowledge base. This approach uses four phases: elicitation, framework definition, information extraction, and formalization. The scope of each stage is described below.

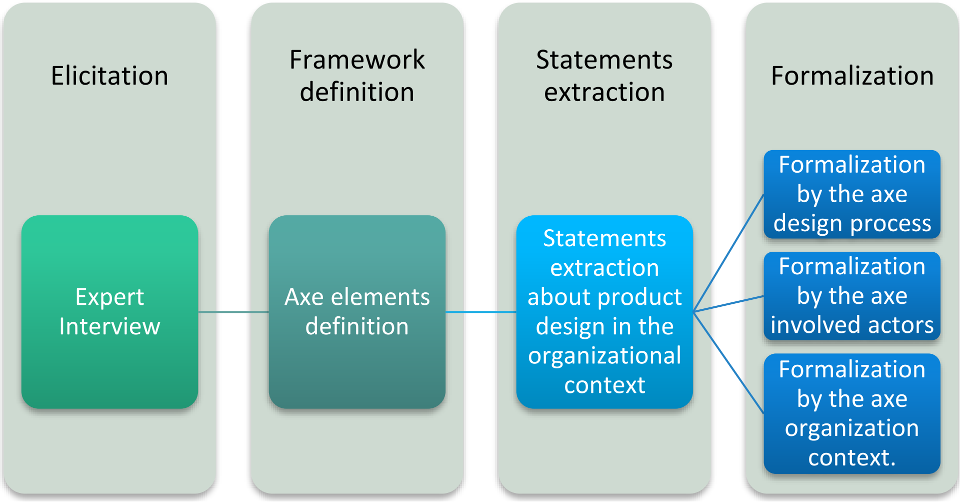

Figure 4-1 Method for the construction of the knowledge base

Elicitation: In this stage information is collected. for this research it was made using the interview protocol described in Table 3-1, having as information source the eleven experts who are also actors in different design teams.

Framework definition: To give a structure for information extraction to construct the knowledge base, an analysis framework is defined based on the results described in Chapter 3. Based on this framework, the following axes will be considered for the analysis: *design stages*, *actors involved*, and *organizational context*. It was found that the different design processes have similarities, but also different elements, i.e., different design stages, actors, and contextual conditions. To be as exhaustive as possible for the definition of the analysis framework, the elements within the axes of design stages and actors are established by including all the identified elements mentioned by the experts from all the analyzed design processes. Additionally, the elements of the axe organizational context are defined based on a variant the business model canvas (Osterwalder & Pigneur, 2010).

Extraction: Information statements expressed by the experts were extracted. The focus was the information considered as implicit (based on their experience and context) and at the same time applicable to different design processes as recommendations for decision-making. Particularities of each of the experts, and personal subjectivities and opinions were screened out. The specific criteria used for statements extraction were:

- Generic information that can be applied by any design team.
- Clear learnings from the expert's experience.
- Conclusions made by the expert comparing two or more design processes.
- Key decision points evident to the expert.

Formalization: Information was formalized by classifying the individual statements extracted from experts according to the defined analysis framework. Each statement was compared to each element of the framework to establish the existence of an interrelation between them (1) or none (0). Additionally, the formalization was validated by our research team, who are also four experts in product design. The procedure of this validation is shown in Figure 4-2. Experts of our research team validated individually the interrelations between the lists of statements and the framework. Then, they performed a Delphi-based group discussion to reach a consensus about the final list (Grime & Wright, 2016).

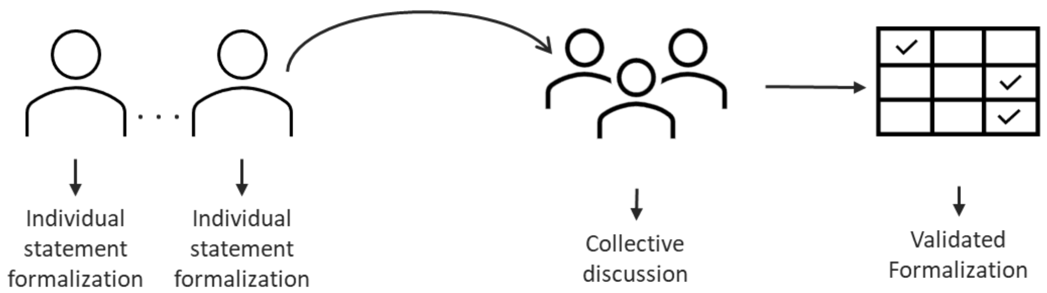

Figure 4-2 Qualitative analysis for the formalization carried out by the research team

4.3 Construction of the expert knowledge base

For the construction of the knowledge base, the list of statements extracted from the experts, the elements defined for each of the axes and the formalization of the interrelation, are assembled as shown in Figure 4-3. It corresponds to the structure of the resulting knowledge base.

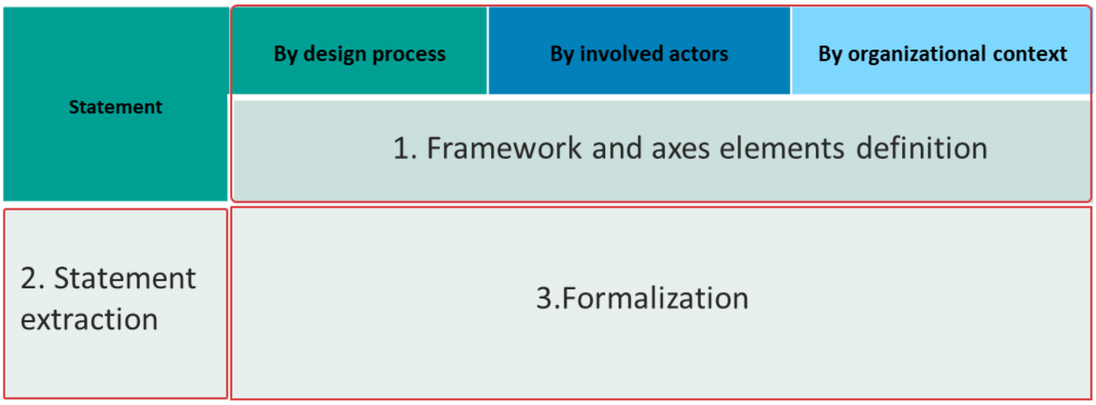

Figure 4-3 General structure of the knowledge base

4.3.1 Framework Definition

4.3.1.1 Elements on the axe design process

The elements of the design process correspond to the design stages mentioned in experts' statements. For their definition, the information collected during interviews and captured in the "*Design Stages*" column of Table 3-2 of each design process was used. All the "design stages" of the eleven product design processes, which were positioned in the first row of Table 3-2 are used here to establish the elements of the axe design process. Each product design process contributes to a certain number of stages define the axe design process of the framework, as shown in Figure 4-4.

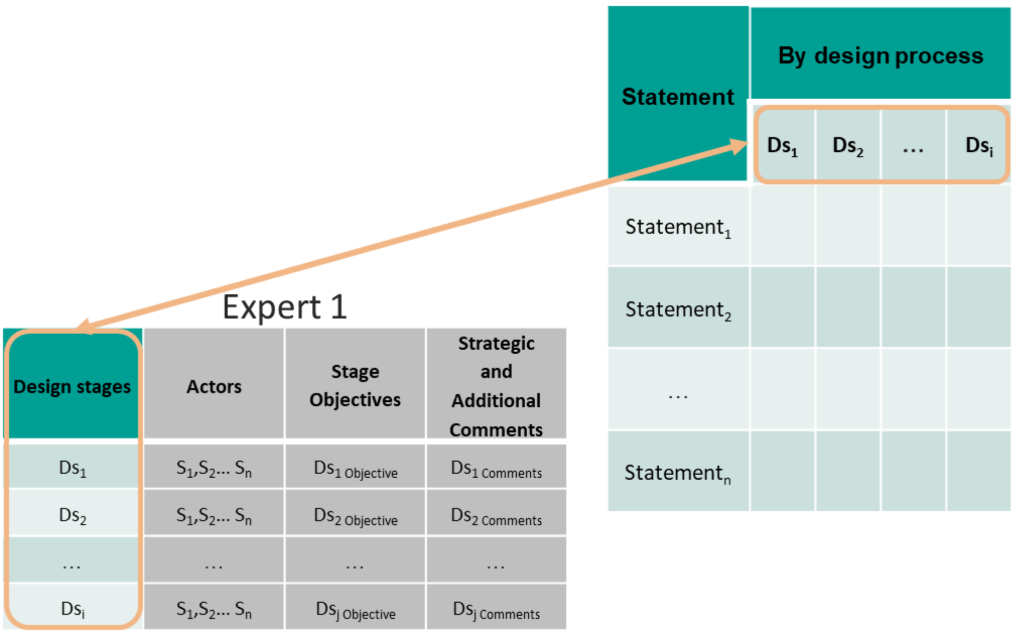

Figure 4-4 Identification of the elements of the design process axe derived from the experts

When adding data from a new expert, the number of categories increased as shown in Figure 4-5. In the case of repeated information, only one of the columns is retained. When analyzing the design stages of the different organizations, the names assigned by each of them may differ from each other despite having similar objectives. Additionally, some companies grouped several stages. Because of this, special attention is given when analyzing repeated or similar design stages to assigning the most general name for each element of the axe reflecting a single objective in the process. At the end of this, a definitive list of design stages was obtained. All stages were kept even if they had only been mentioned by one expert.

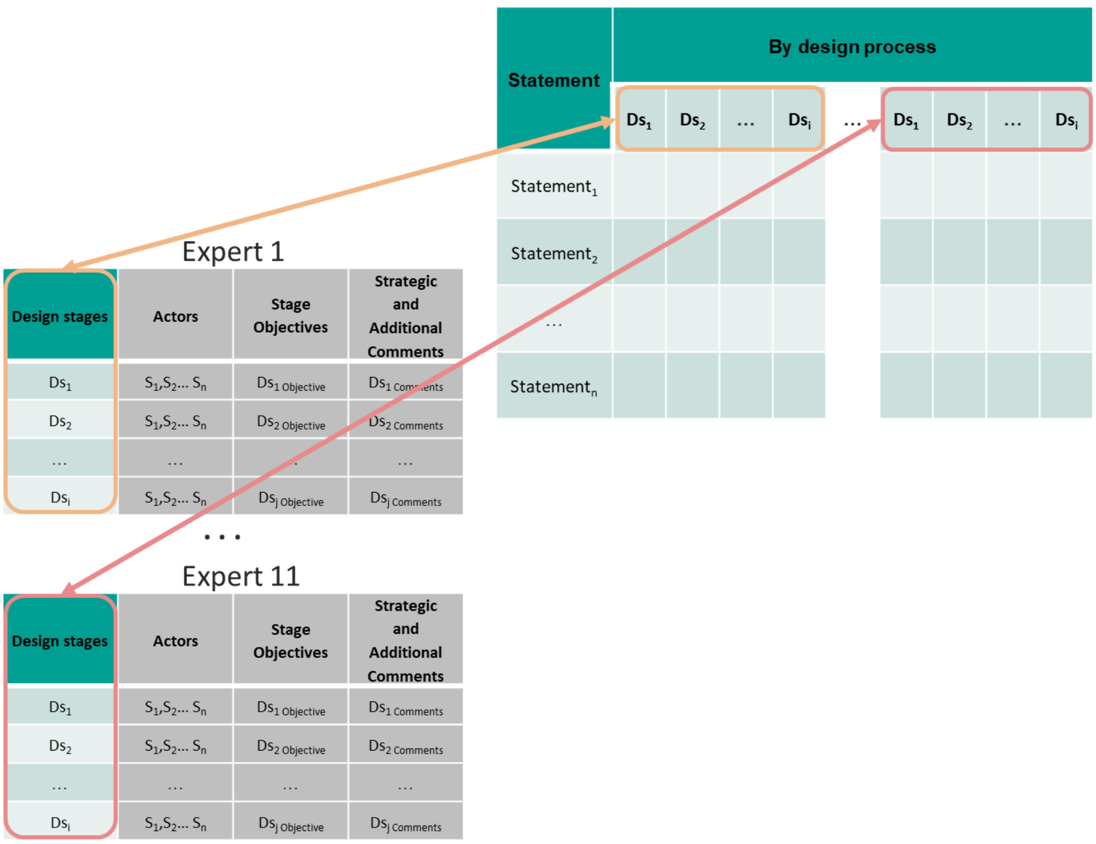

Figure 4-5 Multiexpert data compilation regarding the elements of the design process axe

4.3.1.2 Elements on the axe of actors

The elements definition in the axe of actors makes possible to highlight the relationships between expert statements and the organizational actors that appear in those sentences. For their definition, a similarly data treatment as the one presented for the axe “design stages” is carried out, adding as many rows as necessary according to the actors named by the experts. Figure 4-6 shows how new elements were integrated to the axe.

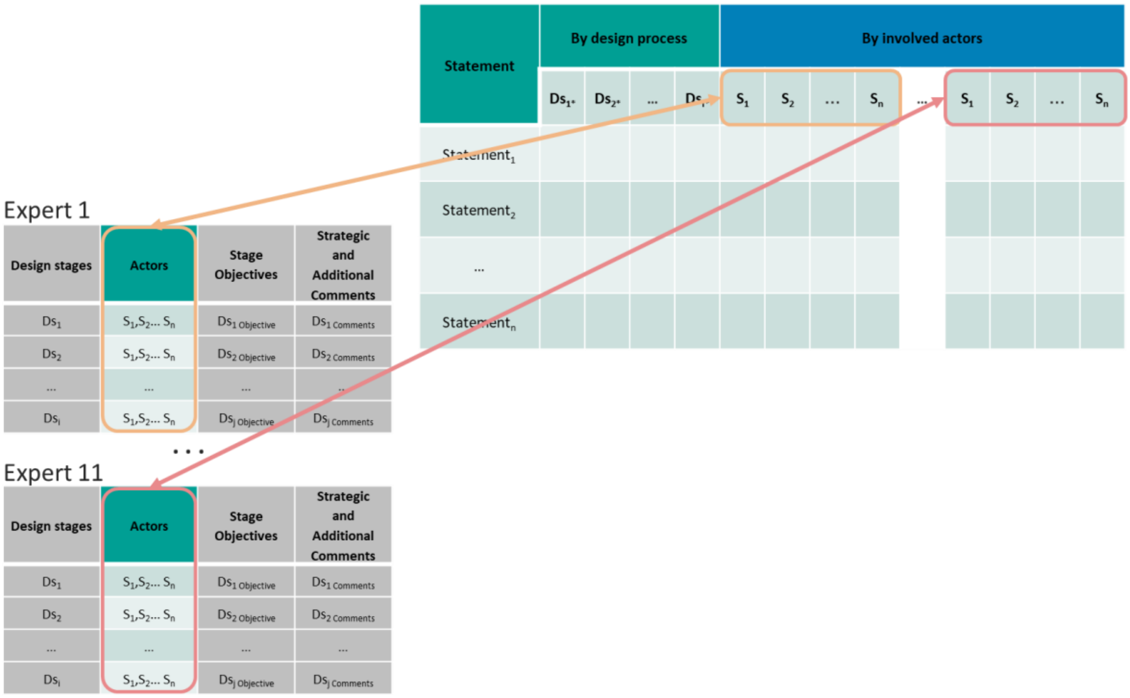

Figure 4-6 Data collection regarding involved actors

4.3.1.3 Elements on the axe of the organizational context

The third axe of the framework focuses on the organizational aspects and the business context. It is proposed using an adapted version of the business model canvas (Osterwalder & Pigneur, 2010), which is a model strategic management template used for new business creation processes. In this case it was used in the analysis of product design processes given that it adequately summarizes many of the key aspects of the organizational context that were discussed in the previous chapters, such as user-centered design, as well as the organizational conditions and resources that exist in the product design system. This adapted model has nine elements:

- Customer segments: This corresponds the target market. Normally, the design team and the organization have well-defined customer segments and focus on identifying and responding to their needs.

- Value propositions: This is the reflection of the organization's strategic directives. It affects the decision-making process in the company, including all stages of product design.
- Channels: The channels of communication with customers refers to the means and resources used in product design to obtain information on the needs and requirements of the target market.
- Customer relationship: This refers to all interactions with the customer. During all the stages of product design and development, the design team can potentially interact with its users, whether for needs analysis, testing and prototype validation.
- Revenue stream: This is the profit and revenue from each of company market segment.
- Key Resources: This groups all organization available resources, including physical, human, and economic, and their effect on decision-making based on them or on the possibility of obtaining them.
- Key activities: This is the product design stages that are well defined and structured, reactive to organizational changes and clear to the actors involved.
- Key partners: the design team establishes who may be potential partners. They expect exchanges of information, services, or products.
- Cost structure: economic considerations of market segments that should be respected throughout the design process.

Complete axe elements compilation

Figure 4-7 shows the complete compilation of the elements of each of the 3 axes of the analysis framework. For the design process axis, 20 descriptive elements were identified. on the other hand, 18 internal or external actors that can play a role in the design of chemical products were identified. additionally, it presents the 9 elements of the organizational axis previously described.

4.3.2 Statements extraction

In this section the extraction of the stamens that are part of the knowledge base is exemplified. The statements extracted from two of the eleven experts is presented. A description of those experts and their roles in chemical product design processes, as well as the statements extracted are presented below.

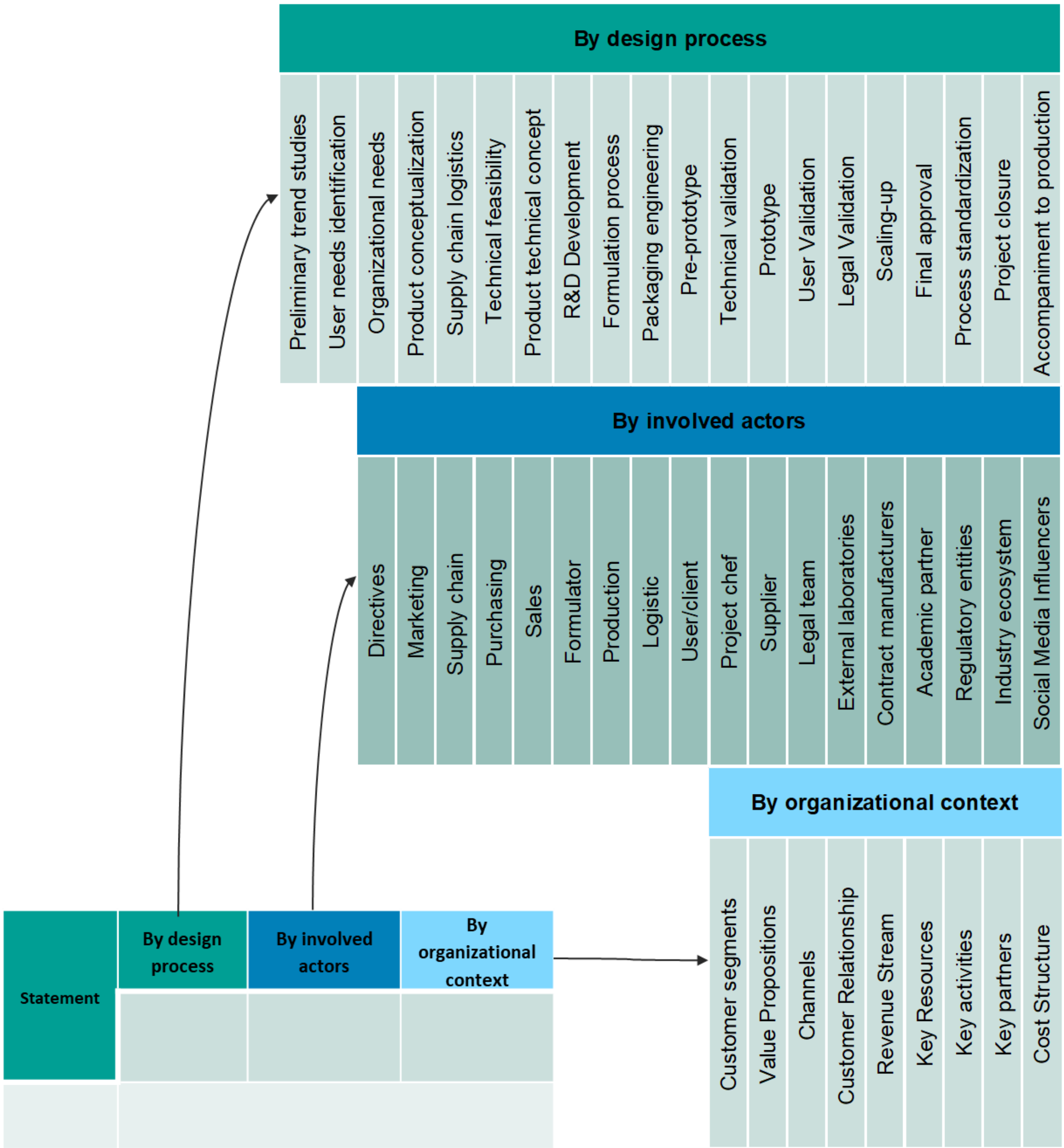

Figure 4-7 Compilation of the elements of the axes of the framework of analysis

Expert 1

The expert shared some experiences as an actor in different roles in a cosmetics company, highlighting a multi-role experience moving from the technical side to management tasks. The expert has been part of teams dedicated to different types of cosmetic products, in the form of emulsions, liquids, and solids. Currently, the expert plays the role of project articulator between the different areas of the organization.

The statements extracted from the interview with this expert are:

- Involve the entire design team in the early design stages.

- Let the formulating team provide inputs throughout the entire design process.
- Be aware of constraints given by access to resources, materials, and technology
- Be clear about the objectives of the project and the regulatory constraints
- Involve the user as quickly as possible to validate the results at different stages of the design.
- Know the structure and functioning of the design team.
- Involve the company's operational logisticians to establish the impact of adding a new product.
- Find key partners in suppliers and service providers.
- Consider the needs that a new product generates for the logistics, warehousing and purchasing areas.

Expert 2

The trajectory shared by this expert corresponds to an entrepreneurial experience based on product formulation. Multiple roles are developed by this expert, from formulation to marketing. This multipurpose role gives the expert a global vision of the aspects related to the creation of new formulated products, including the relationships established with customers, suppliers, and service providers. The statements are:

- Feed your design process with information from market trend analysis and strategic business objectives.
- Establish initial contact with your suppliers to assess the feasibility of your product concepts. Don't forget the local context of your suppliers.
- Offer product alternatives based on the local context of your consumers.
- Simultaneously adapt your design process to regulatory updates.
- Generate quick prototypes to test with users, even if it is not a final formulation.
- Consider production capacity, packaging restrictions and logistics to move to a final formulation.
- Work with third party contractors when scaling up production at the factory, maintaining quality controls.
- Find allies in contractors, suppliers, and distributors.

The complete list of statements extracted from the eleven interviews with the experts is presented in Appendix B in Table B-1

4.3.3 Statement formalization

In this section all the extracted statements (section 4.3.2) are analyzed according to all the elements of framework (section 4.3.2). When an interrelation between a statement and an element of the framework is found, it is highlighted with a 1 in the formalization matrix. This process is illustrated below by analyzing two statements with all the elements of the framework. The formalization matrix together with the statements and the framework constitute the knowledge base proposed in this chapter.

Considering the first statement of the expert one in the example presented in section 4.3.2: *"Involve the entire design team in the early design stages",* the analysis is the following:

It is a general statement corresponding to a recommendation for different organizations. When analyzing it in relation to the design process, it mentions that it should be applied to the initial stages. Thus, the statement is concerned with the initial design stages of the axe design process, from preliminary stages to product conceptualization. In relation to the actors, it refers to all the internal team of the organization. Thus, regarding the actors' axe, the statement is related to all the representatives of the internal areas of the organization. With reference to the organizational context, it is considered as related to a key activity in the design process. Table 4-1 summarizes the characterization for this statement (only the elements with a 1 are shown there).

Table 4-1 Example 1 of expert statement formalization

	By design process				By involved actors										By organizational context
Statement	Preliminary trend studies	User needs identification	Organizational needs	Product conceptualization	Directives	Marketing	Supply chain	Purchasing	Sales	Formulator	Production	Logistic	Project chef	Legal team	Key activities
Involve the entire design team in the early	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1

design stages.															

As a second example, the characterization of the first statement of the second expert: *"Feed your design process with information from market trend analysis and strategic business objectives",* is as following.

In this case this statement contains more specific information than the statement of the previous example. For the analysis from the design process axe, the design stages related to market research and the analysis of the users and the organization needs are highlighted. Two key actors are identified: the organization's management are, which must transmit its strategy to the design team, and the marketing area, in charge of studying the market and users. In relation to the organizational context, this statement is related to two categories: key activity of the design team and the value proposition by requiring clear information on the organization's strategy. Table 4-2 shows the characterization this statement.

Table 4-2 Example 2 of expert statement characterization

	By design process			**By involved actors**		**By organizational context**	
Statement	Preliminary trend studies	User needs identification	Organizational needs	Directives	Marketing	Value Propositions	Key activities
Feed your design process with information from market trend analysis and strategic business objectives.	1	1	1	1	1	1	1

The complete analysis of all statements is the knowledge base proposed in this chapter. Figure 4-8 shows a sketch of the knowledge base matrix that gathers the three analyzed axes: design process, actors, and by organizational context, and formalize the statements in it. The complete knowledge base is presented in the Appendix B in Table B-2.

Statement	By design process				By involved actors				By organizational context								
	1.Preliminary trend studies	2.User needs identification	...	20.accompaniment to production	1.Directives	2.Marketing	...	18.Social media influencers	Customer segments	Value Propositions	Channels	Customer Relationship	Revenue Stream	Key Resources	Key activities	Key partners	Cost Structure
Statement$_1$	1				1									1			
Statement$_2$					1					1					1		
Statement$_3$		1				1							1		1		
...																	
Statement$_n$	1			1						1			1				1

Figure 4-8 Knowledge base matrix sketch.

4.4 Chapter conclusions

This chapter describes a knowledge base approach to represent the implicit knowledge of chemical product design experts. The method consists of four parts: gathering firsthand information; establishing a framework for analysis; extracting statements concerning the chemical product design process; and characterizing those statements with respect to the previously established framework. The consolidation of these four elements allows us to present knowledge base available information to be used by organizations to analyze their product design process.

Knowledge characterization approach related to the chemical product design process in a business context, presented here, considers multiple elements of different dimensions of the product design system. This data processing allows us to perform an organized knowledge representation, eventually this representation can be useful to exploit implicit knowledge in product design. In addition, the knowledge representation can give a broad vision to both the design team and the management directives. Knowledge characterization approach permits to have a closer and more realistic picture of the product design process requirements according to experts.

The knowledge base presented is the result of a collective participation of experts and the research team. It is essential that it be disseminated to the community in general concerned by the design of chemical products, this would consolidate its acceptance as a descriptive instrument of the product design system, in addition to being tested in a real situation to establish whether it meets its objective as well as its ability to adapt and evolved in different contexts.

The method for knowledge base creation presented in this chapter can be used in other domains with different contexts and can be used by organizations to store and organize implicit knowledge acquired through experience. The use of the knowledge base can be useful for problem solving in organizations, since it allows the managers to access to formalized and categorized information, the statements in this case will act as recommendations or considerations to be considered to act and intervene in design processes. The knowledge base is susceptible to be fed with fresh information from new actors and experts, until it becomes a robust system.

Finally, this knowledge data base will be valorized through the development of a design product management recommendation tool. Considering that the knowledge base is a first version of the formalization of the know-how of project leaders, the following research step consists in proposing a tool giving recommendations to formulators. More, precisely, the aim is to describe the current design process of a company and analyze if the application of some knowledge integrated in the data base will help improving this current process.

5 Construction of a tool to support the management of the chemical product design process

This chapter presents the design and implementation of a tool to support decision-making for the management of the chemical product design process within organizations. The tool aids to formalize and analyze the product design system of an organization and proposes recommendations for its improvement according to its value creation concepts, strategy, and business model. The evaluation of the design process is done in collaboration between the researchers and the actors of the organization. The recommendations for the eventual improvement of the design process are proposed using the knowledge base presented in Chapter 4.

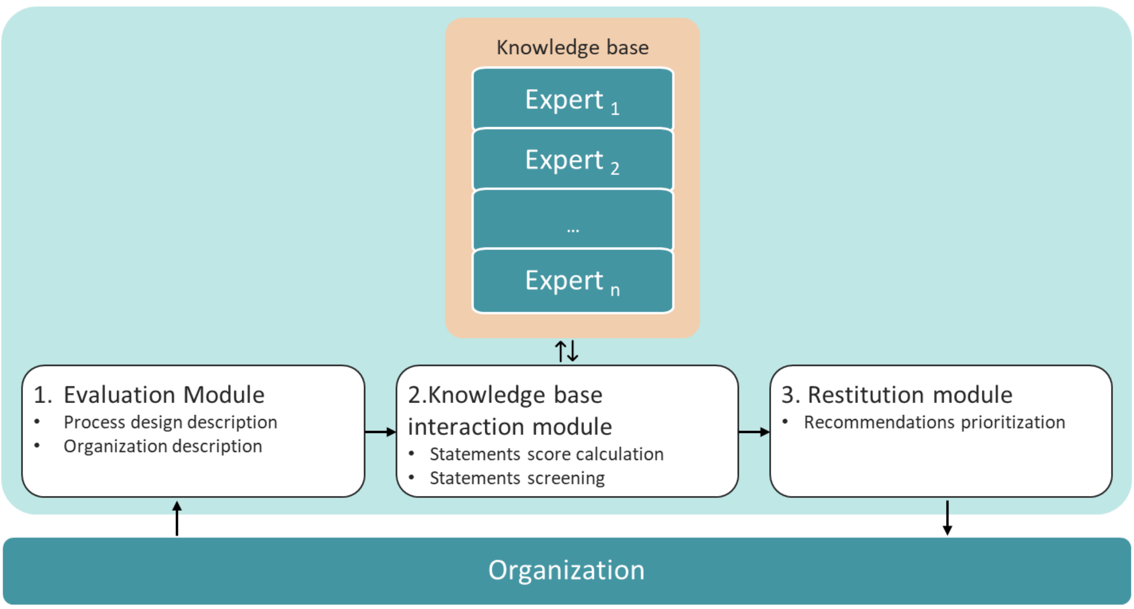

Figure 5-1 Operational deployment of the support tool

As shown in Figure 5-1, the tool has three components: an evaluation module, where the analysis of the actual organization's design process (ODP) and the establishment of the organization profile are carried out. A recommendation module, where the evaluation results are compared with the knowledge base allowing the organization to identify recommendations responding to its organizational goals. And finally, a restitution module that enables the proposition of the recommendations to the organization and their analysis by the members of the design teams for their implementation. The modules are described in detail in ethe following sections.

5.1 Evaluation module

In this module both, the design process, and the organization are analyzed. The analysis is done considering that, as concluded in chapter 3, the product design process is specific to each organization, thus it must be assessed also considering the company profile. Additionally, the evaluation is made in collaboration between the external observers (researchers) as well as by the company's internal actors represented here as the design team members. Moreover, more than one actor is invited to take part in the evaluation to generate a multi-perspective and broader picture of the design process.

5.1.1 Process design description

Information on the organization's design process is collected through direct contact with multiple design team members using two methodologies: semi-structured interviews and a workshop. Information is individually collected in the interviews to map the different perspectives of the design process. Then, a workshop is conducted to enable actors to complete and formalize collectively the actual design process of the company. Figure 5-2 represents this procedure. Each of the phases are described following.

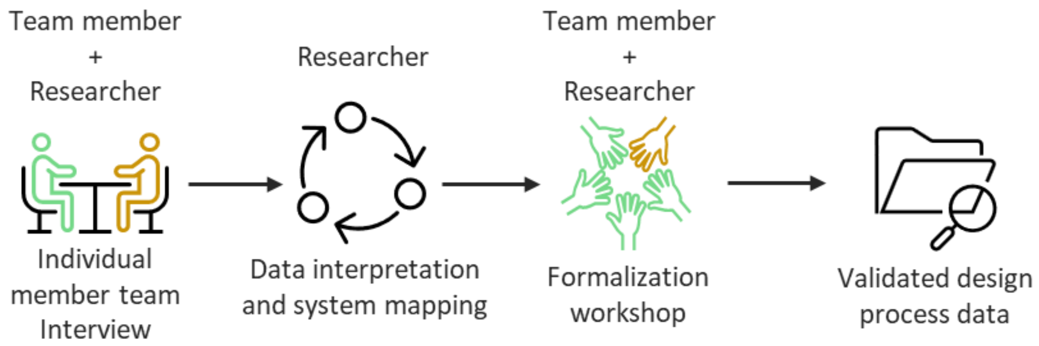

Figure 5-2 Procedure for the description of the product design process

5.1.1.1 Individual member team interviews

The first contact with the actors involved in the design process, as well as the acquisition of initial data, is conducted through individual interviews with the design team members. The purpose of the interviews is to capture information about the product design process as expressed independently by each design team member and to generate a map of each vision of the process. The interview protocol was divided in three parts: a presentation explaining the goal of the interview, a semi-structured interview to know the profile of the participant, and a semi-structured interview to map the design process from every point of view. The interview protocol was proposed to fit the role of each team member The general guidelines of the interview protocol are presented below. The complete protocol and material used for the interviews can be found in the Appendix C.

Protocol guidelines:

- To identify each team member's profile and experience.
- To know in detail their role, responsibilities and performed activities related to the design process.
- To ask for a detailed description of the company's design process, highlighting the interviewee’s vision of the process.
- To understand the interactions between actors during the decision-making process in the different design stages.
- To know the effects of the organization's strategy on the product design process.

5.1.1.2 Data interpretation and mapping

The analysis of the information shared by the interviewees is done based on the same criteria presented in chapter 3, Table 3-2 (also used for the creation of the knowledge base). Thus, the stages of the design process, the actors involved in each stage, and the organizational strategy influencing the design process are identified. Additionally, the individual mapping of the product design process also contains the *intermediate design objects* (IDO) of each design stage. IDO are concrete objects that represent the design activity and support for the design team's coordination (Elias & Chaumon, 2022). Examples are sketch, product data sheet, commercial pitch, technical drawing, prototype, as well as digital elements such as e-mails, meeting reports, among others. The identification of IDO is fundamental to map the actual product design process because they constitute tangible traces and concrete objects produced, discussed, and circulated between actors during the design process.

Figure 5-3 shows the results of the individual interviews. There, an individual table is filled in for each team member, thus several maps of the design process are made, each containing a different point of view of the same process. The results are shown in several tables representing the product design system according to of each one of the team members.

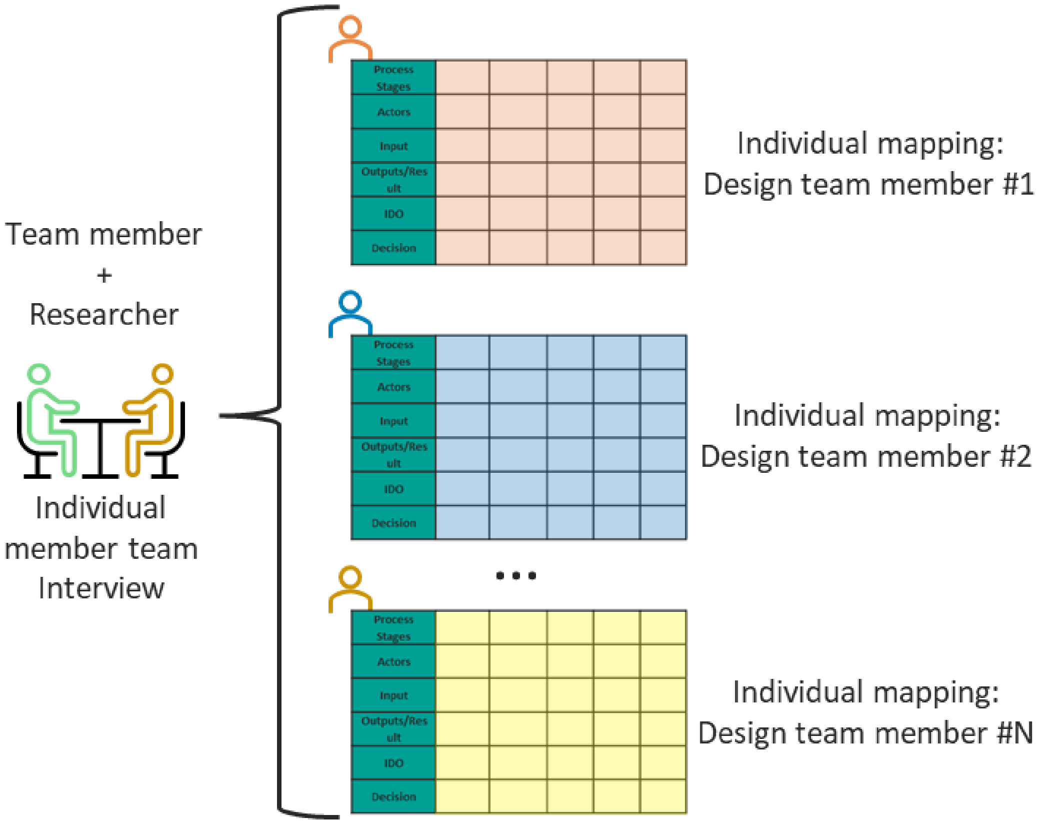

Figure 5-3 Individual product design system mapping

The set of tables from Figure 5-3 are then summarized in a single table (Table 5-1) containing all the visions of the product design. Table 5-1 contents all the individual visions of the members of the design team, respecting the names and characteristics assigned by each of the members and unifying those that are similar. The summary is color-coded to show which team member each version corresponds to. This table is the input for the discussion that takes place in the workshop.

Table 5-1 Summary table of the product design system mapping of all team members. (Team member 1, …, Team member N°)

	Stage 1	Stage 2	… Stage N°
Stages of the Process	• Stage name according to design member 1 • … • Stage name according to design member N°	• Stage name according to design member 1 • … • Stage name according to design member N°	• Stage name according to design member 1 • … • Stage name according to design member N°
Actor	• Involved actors according to design member 1 • … • Involved actors according to design member N°	• Involved actors according to design member 1 • … • Involved actors according to design member N°	• Involved actors according to design member 1 • … • Involved actors according to design member N°
Inputs	• Input according to design member 1 • … • Input according to design member N°	• Input according to design member 1 • … • Input according to design member N°	• Input according to design member 1 • … • Input according to design member N°
Outputs/ Result	• Results according to design member 1 • … • Results according to design member N°	• Results according to design member 1 • … • Results according to design member N°	• Results according to design member 1 • … • Results according to design member N°

5.1.1.3 Formalization Workshop

To finish the evaluation module, an integration of the different visions of the design process is carried out through a collaborative workshop with the participation of the interviewed design team members. This is done with the aim of generating a single agreed-upon map of the design process of the company. In the collaborative workshop the team members analyze all the versions of the design process that were identified during the interviews and discuss about them to stablish a unique version (as represented in Figure 5-4). This version corresponds to the current and consensual product design process of the company. It contains the design stages, the inputs and outputs of each stage, the actors, the IDO and the decisions to be made at each stage.

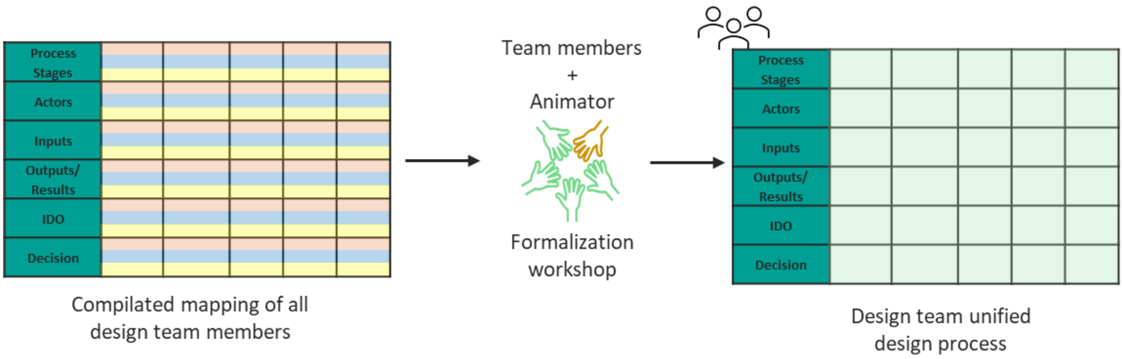

Figure 5-4 System mapping formalization workshop approach

During the workshop, the summary table (Table 5-1) with the different versions of the design process is presented to the design team members, together with a modifiable board containing an empty table with the analysis criteria. The members of the design team are invited to discuss the different versions of the design process stage by stage and to stablish agreements that must be represented in the board. This board allows the participants to move/modify/delete/add elements to define a unified design process in a participatory dynamic as shown in Figure 5-5. The objective of this process is to formalize the design process by consensus. The generic material to prepare this workshop is presented in Appendix C.

Figure 5-5 Design process unification workshop board

5.1.2 Organization description

Organization profile

The organization profile of the company is carried out by the research team using the information collected in the interviews and the formalization workshop. A profile of the organization is created to generate recommendations adapted to the company in a later analysis stage. The profile is done based on the characterization of the organizational context, using the elements on the axe 'organizational context' of the knowledge base (section 4.3.1.3). The company profile is scored according on how well its design process reflects the intentions of the elements. Each element is evaluated by the research team on a five point scale (Jebb et al., 2021) as shown in Table 5-2.

Table 5-2 Profile qualification assessment

	Strongly disagree (1)	Disagree (2)	Neutral (3)	Agree (4)	Strongly agree (5)
Customer segments: Does the design process have well-defined customers segments and respond strictly to their needs?					
Value Propositions: Does the design process consider the value proposition in all its stages and decisions?					
Channels: Are the communication channels with partners and customers clear during the entire design process?					
Customer Relationship: During the design process stages, does each member of the design team know the needs of the users?					
Revenue Stream: Are the methods to achieve profit and incomes considered in the design process?					
Key Resources: Does the design process focus its efforts based on its resources or the ability to obtain them?					
Key activities: Are the design process activities clear? Do the design process activities have well-defined objectives and outcomes?					
Key partners: During design process, are the current and potential partners identified as resources?					
Cost Structure: Is the cost a major constraint during the decision-making process?					

Key points identification

In addition to the company profile, company weaknesses or key critical points of the design are also identified. This is done considering the individual interviews and the collective workshop about the design process. Based on this, it is possible to identify points of inflection or discomfort among the actors throughout the stages of the process. These points are aspects to work by the design team.

5.2 Knowledge base interaction module

The objective of this module is to derive recommendations from the knowledge base that respond to the specific design process and organization profile. For this, the consensual design process (Section 5.1.1), the organization's profile, and the key points identified (Section 5.1.2) are used in combination with the knowledge base (Chapter 4). This is done in two steps: *1) statement score calculation according to company profile,* where the statements of the knowledge based are scored to select those that better fit the company profile and 2) *statement screening according to the design process*, where the statement impacting the process stages where there are concerns (key points) are selected.

5.2.1 Statements score calculation according to company profile

Based on the information represented in the *organization's profile*, all statements in the knowledge base are scored to select those that are most adapted to the company. This calculation is programmed in a spreadsheet and is developed as shown below:

a) Calculations of the statements individual vector from the knowledge base: The knowledge base developed in the Chapter 4 has the form of a matrix as shown in Figure 4-8. For each statement, the section containing the elements related to the organizational axis are named here as the *statements individual vector* (SIV_n described in Equation 5-1). The SIV_n of each statement contains 9 elements already defined in the knowledge base that indicate if the content of the statement has a relation to the organizational axis (scored with 1), or not (scored with 0). Figure 5-6 shows an example of how the SIV_n is extracted for an statement. This is done for all statements in the knowledge base.

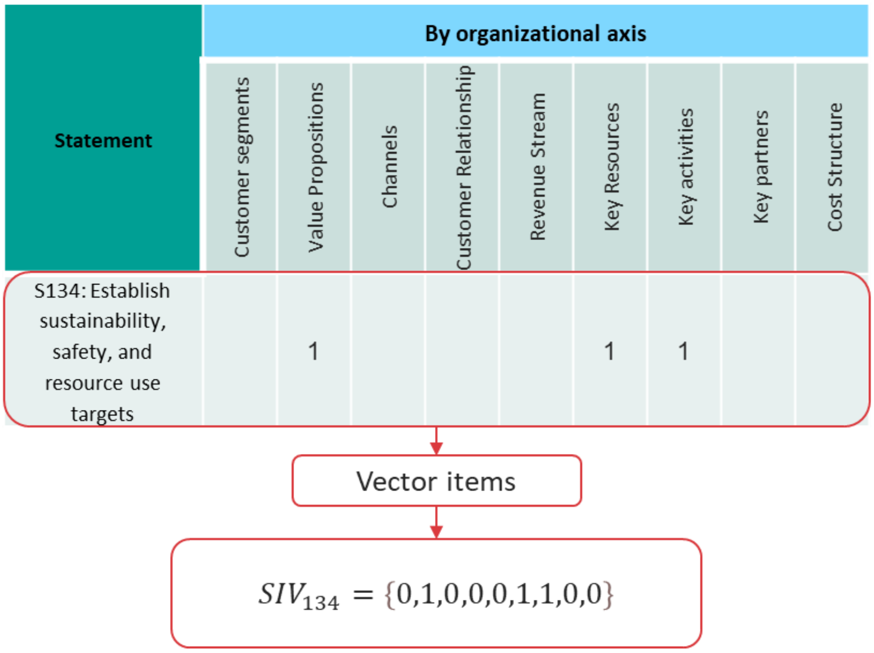

Figure 5-6 Example of qualifying items and characteristic vector for statements

As result, the number of these vectors will be as many as statements in the knowledge base (134 statements from 11 experts consolidated at the time of the writing of this document, available in Appendix B.). The values within the *statements individual vector*s were already established in the knowledge base in Chapter 4. Their values are not modified unless the knowledge base is altered.

Equation 5-1 Configuration of the statement characteristic vector

$$SIV_n = \{Q_1, Q_2, Q_3, Q_4, Q_5, Q_6, Q_7, Q_8, Q_9\}, \text{ where } Q_{1\ to\ 9} \text{ takes value 1 or 0}$$

b) Definition of the organization improvement vector based on the organization profile: The organization improvement vector (OIV_n) is calculated based on the organization profile (described in the section 5.1.2). The organization improvement vector prioritizes the elements of the organization profile to work on, i.e., the elements with the lowest score in the profile. For this, it is considered that the ideal score of each element of the company profile should be equal to 5 (maximum score - Table 5-2). Then, the organization improvement vector (OIV_n) is calculated by subtracting the company profile vector from a vector of 9 elements with the ideal value as shown in Equation 5-2. Table 5-3. shows an example of a company profile vector (Third column) and the respective Organizational improvement vector (Fourth column).

Equation 5-2 Calculation of the *organization improvement vector*

$$OIV_n = V_{ideal} - V_{company\ profile}$$

Table 5-3 Example of profile rating and Organization Profile Vector

By organizational context	Ideal value vector	Organization profile	Organizational improvement vector
Customer segments	5	2	3
Value Propositions	5	1	4
Channels	5	2	3
Customer Relationship	5	2	3
Revenue Stream	5	3	2
Key Resources	5	3	2
Key activities	5	4	1
Key partners	5	5	0
Cost Structure	5	4	1

The Organizational improvement vector is described by a column vector of 9 elements as shown in Equation 5-3.

Equation 5-3 Configuration of the *Organizational improvement vector*

$$OIV_n = \begin{Bmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \\ R_5 \\ R_6 \\ R_7 \\ R_8 \\ R_9 \end{Bmatrix}, where\ R_{1\ to\ 9}\ \ takes\ value\ of\ 0{,}1{,}2{,}3\ or\ 4$$

c) Statement impact score calculation: A score for each statement is calculated considering two aims criteria: 1) to prioritize those statements that concern the greatest number of elements of the organizational analysis axis, and 2) to consider those elements of the profile that the organization needs to focus on the most. To do that, a statement score (S_n) is calculated for each statement in the knowledge base. This is done using Equation 5-4 where the dot product between the *SIV* (Equation 5-1) and the *OIV* (Equation 5-3) is calculated. Statements with higher score are related to more elements of the organization's axis and better correspond to the improvement needs according to the company's profile.

Equation 5-4 Calculation of statement scores

$$S_n = SIV_n * OIV_n$$

$$S_n = Q_1R_1 + Q_2R_2 + Q_3R_3 + Q_4R_4 + Q_5R_5 + Q_6R_6 + Q_7R_7 + Q_8R_8 + Q_9R_9$$

As example, taking the statement #134 (the same in the Figure 5-6), the score is calculated using the company profile (in the example of Table 5-3):

$$S_{134} = 0*3+1*4+0*3+0*3+0*2+1*2+1*1+0*0+0*1 = 7$$

The definitions of the *SIV* and the *OIV,* followed by the score calculation, lead to a ponderation that prioritizes the knowledge base statements in a customized way according to the profile of the organization involved.

5.2.2 Statement screening

Once all the statements available in the knowledge base have been scored, only those recommendations adapted to the company key points and design process are selected. For this, the stages of the design process where *key points* were found are identified. And only those statements that concern those design stages are selected. As result, a selection of statements corresponding to the design stages of concern and scored according to its adaptability to the company are obtained as shown in Figure 5-7. Additionally, the actors most closely related to these recommendations and therefore most involved in the implementation of the recommendations are also identified.

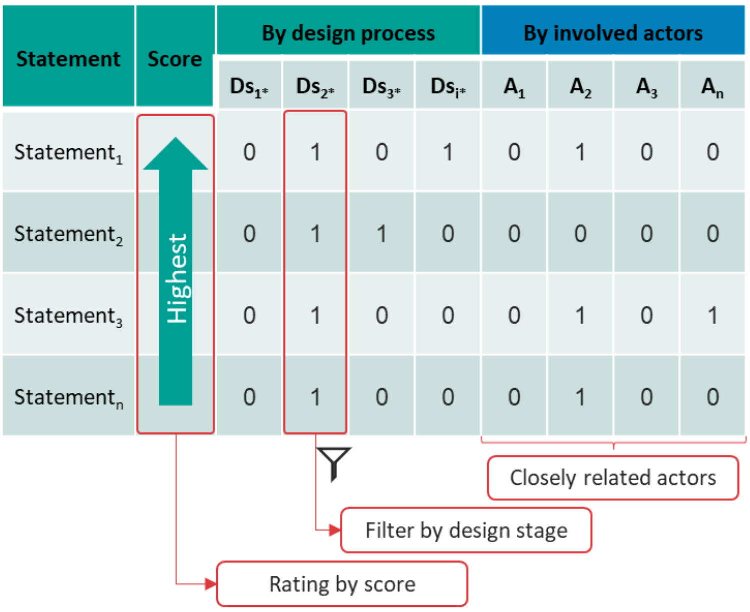

Figure 5-7 screening of statements according to design stages criteria

The combination of the recommendations scores and the filtering strategy by design stage gives pertinence to the recommendations of the tool. The group of recommendations obtained can include more than one design stage (depending on the evaluated key points), reason why the research team should select recommendations, avoiding repetitions and giving a global vision.

5.3 Restitution module: prioritization and implementation of the recommendations

Based on the profile of the organization and the formalized product design process, the most relevant suggestions of the knowlwedge base are selected. Those recommendations (statement application)are presented to the design team, who has to evaluated them according to its ability to create value(improvements in various aspects for the consideration of the design team) in the organization and its feasibility for their prioritization (Brunet, 2019).

The prioritization of statements is done in a collective workshop with the design team members. There, the most suitable recommendations are returned and analyzed by the design team using the prioritization grid presented in Figure 5-8. Recommendations are localted considering their behavior in the two axes of the figure: value creation and feasability, according to the capabilities and ambitions of the companie . The figure has four quadrants allowing the arrengement of the selected recommendations in the following categories:

- *High impact and low effort (top-right):* recommendations that are simple to implement or present a low-cost in their execution and, in addition, generate a favorable impact on the design process.
- *High impact and high effort (top left)*: recommendations that involve significant efforts to be implemented, but their impact on the design process can be considerable.
- *Low impact and low effort (bottom right)*: recommendations that do not generate a large impact on value generation but are easily achievable even without investment of resources.
- *Low impact and high effort (bottom left):* recommendations that require a significant investment of resources and do not have a clear or significant impact.

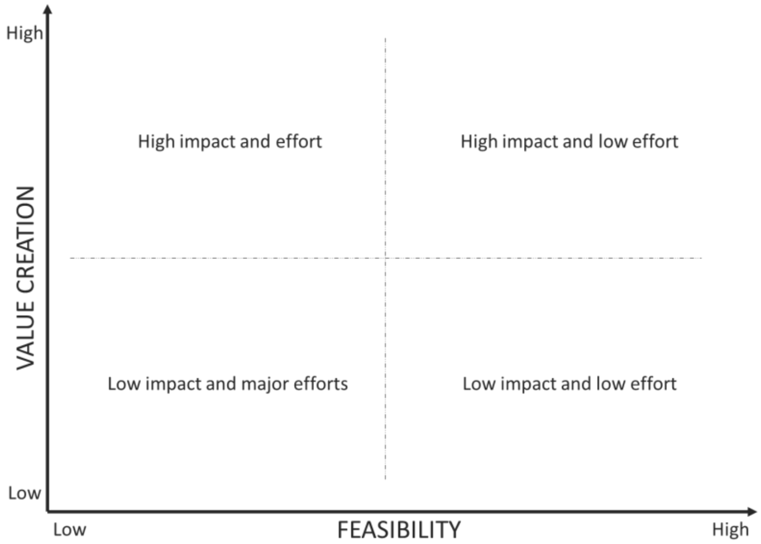

Figure 5-8 Recommendation prioritization grid

In order to enrich the discussion around the recommendations, different value creation criteria can be established depending on the strategy of the company. For example, a company whose goal is to produce in a more sustainable way, can evaluate recommendations according to its ability to generate value relate to sustainability. The evaluation of the recommendations considering different concepts of value of interest for the company (relation with the customer, sustainability, originality, etc.) allows to exploite their potential at diferente leves and to discuss about the perspectives of the future process of the organizationas shown in Figure 5-9

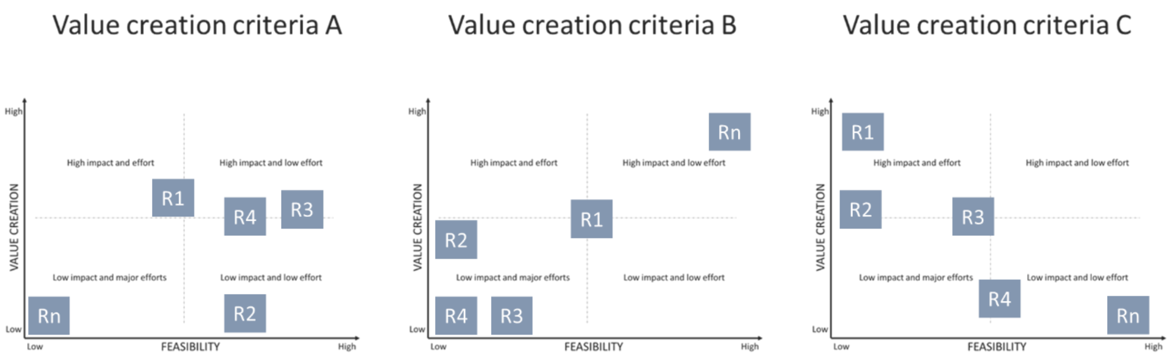

Figure 5-9 Result of prioritization of recommendations with value-creation criteria.

Recommendations that the company could implement are those that will lead to high value creation. The simplest and first to be implemented are those located in the upper right quadrant of the value charts.

The implementation of the recommendations implies changes in the company's current design process. They may lead to the introduction of intermediate design stages (which are not considered in the current process) or to the inclusion of new stakeholders, or the participation of actors in other stages in which they did not participate before (Figure 5-10).

The tool presented here therefore allows companies to generate new methodologies to design their products adapted to their own organizational contexts and issues. This is developed in more detail in the case study presented in chapter 6.

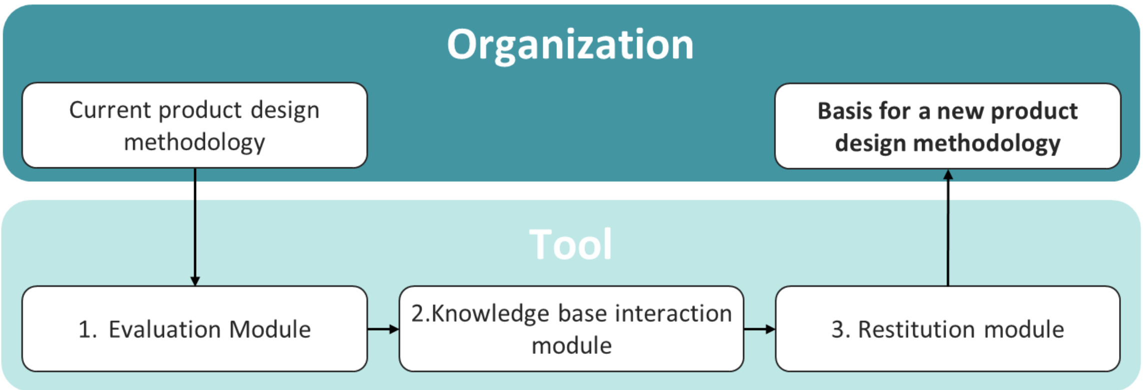

Figure 5-10 Operational deployment of the support tool

5.4 Chapter conclusions

In this chapter, a tool that allows an organization to propose recommendations their chemical product design processes is proposed. The method is participatory, and members of the design team collaborate actively in the identification and evaluation of the recommendations. The tool comprises three modules: the first, to know the current state of the organization design process, the second, to extract recommendations for the improvement of the design process from the knowledge base, and the third, to assess the relevance of the recommendations. Figure 5-10 summarize the integration of the three modules for their application with the objective of generating new design processes that increase the organization's value generation.

6 Experimental test of the tool

The objective of this chapter is to show the tool proposed in Chapter 5 through a case study corresponding to the assessment of a cosmetic company who usually design chemical products. As previously shown, the tool was carried out in several stages, integrating theory and expert knowledge. To further develop the proposal, it is necessary to evaluate its applicability in a real organizational environment. In this evaluation different aspects of the use of the tool in a real context are explored. Aspects such as its adaptability to various setting of actors and projects, its ease of use, as well as its application in decision making processes and design management. Accordingly, it was found that a case study approach is a suitable methodology for this situation (Yin, 2018).

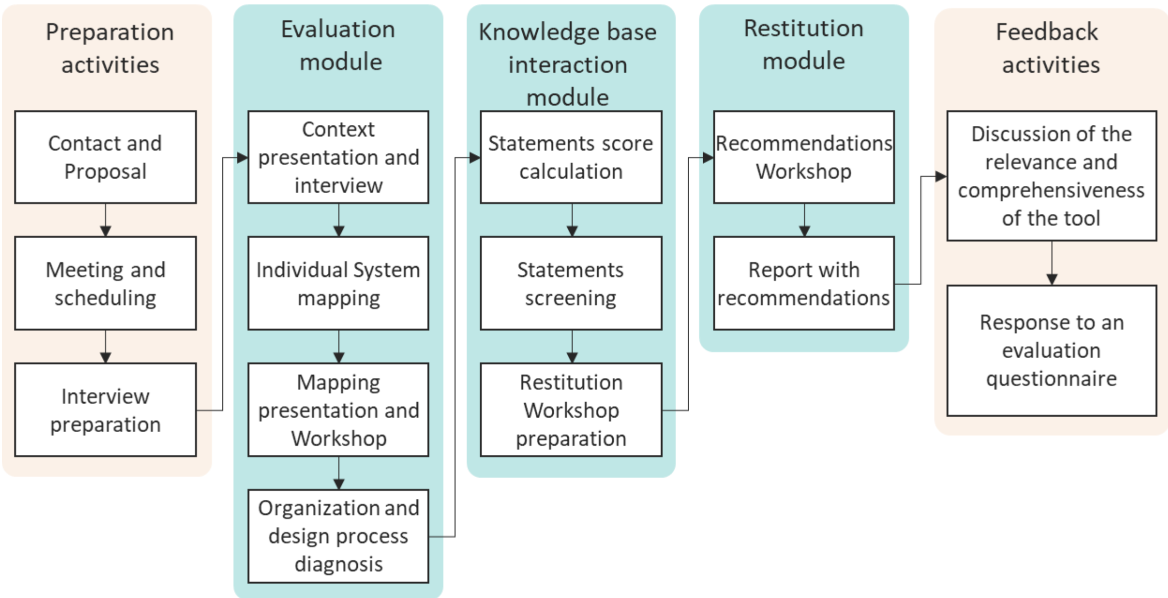

Figure 6-1 Detail of the application of the tool in a company

The objective of the assessment using the tool is to provide the organization with recommendations for the value generation in their own product design methodologies. At the same time, the assessment allows the organization to formalize its design process and to align it with its strategy or business model. Figure 6-1 shows an outline of the steps carried out for the application of the tool. The procedure for its application it is done following the structure of the three modules presented in the previous chapter (5). In the following sections the procedure implementation is described module by module, starting with a brief description of the company where it is applied.

6.1 Selection of the case study

For the application case study, small size cosmetic companies with a design team and a production site in France were contacted. A company of Asian origin with a subsidiary in France was finally selected because of the high willingness of its actors to actively participate in the assessment. The parent Asian company was founded more than 100 years ago. Although it started as a dye production group, the company dabbled in various disciplines, including chemistry and pharmacy as a reseller. Over the years, it evolved into a group covering many fields of industrial production. Today, electronic components and pharmaceuticals and cosmetics are the main business units. The subsidiary was established in France 30 years ago, acting as a chemical distributor. It recently acquired a local production side and started to design and develop products in France for the cosmetic and pharmaceutical sector.

The cosmetic business line is composed of a small group of actors, who design and develop the products in a B2B model and supported by the resources of the multinational organization and the local production side. They also collaborate intensively with academic institutions. Additionally, regarding its experience as distributor, the company has built up an extensive marketing network that allows it to access global markets, mainly in Asia. This network also allows the company to have access to a wide customer network. Among their most recent projects, the production of high value-added cosmetic ingredients which are premixes (formulations ready to be added to a product) with ecologically sustainable ingredients is highlighted.

6.2 Evaluation module

6.2.1 Process design description

Individual interviews and data mapping

As explained in Chapter 5, the evaluation comprises several steps. First is the individual interviews with several actors involved in the company's design process to map the process from different perspectives.

Three actors participating in the design process were interviewed online: the business development manager, the project manager and the academic/technical partner. The latter deals directly with the formulation and product characterization tasks. Table 6-1 shows a list of the actors interviewed and a brief description of the role the actor plays. All the actors have a technical profile, even though not all of them perform technical tasks; this characteristic allows the team to communicate effectively among them. This table also presents the color coding used to represent the design process individually.

Table 6-1 Actors involved in the design process and the role played in it.

Actor	Actor description	Code color for mapping
Business development manager	The actor performs tasks related to the establishment of relationships with the network of customers, suppliers, and partners. He makes a permanent monitoring of the market trends and of possible new customers. He oversees the financial monitoring of the cosmetic division of the organization. He has also a technical profile, although working transversally in the organization and in the design team,	
Project manager	A dedicated staff member dedicated to the management of design and development projects within the organization. He is the leader of the design team, i.e., he oversees communication inside the team.	
Academic partner	This partner is composed of different experts in an academic and research center. It is not part of the organization, but there is a person who leads the formulation projects specifically dedicated to the company. The academic partner has physical resources, such as laboratories and supplies, as well as expertise in different areas, such as cosmetics, biology, statistics, among others. For the mapping exercise the person dedicated to the company projects was interviewed in representation of all the academic partner.	

In Table 6-2, the summary of the three visions of the design process is presented. The collected data included: the design stages, the relationships between the actors, the sources of information, the resources needed to carry out each design stage, and the expected results of each stage. From the collected information, it can be highlighted that each of the actors has its own vision of the process. Thus, the names of the design stages are in some cases different among them. Moreover, in other cases there are design stages not mentioned by all the actors. It is also noted that although the academic partner is not part of the company, it is present in most of the stages and plays a central role concerning technical decisions. Table 6-2 is the basis for the discussion in the formalization workshop with the design team.

It is noted in Table 6-2 that the design team members discuss "distribution mode" and "production mode", two modes in which the organization designs products, this issue will be further reviewed in the formalization workshop.

Formalization workshop

As shown in Chapter 5, the formalization of the design process is developed through a workshop with the participation of the members of the design team. There, the participants were asked to discuss the different visions of their design process (presented in Table 6-2) with the aim of arriving at a consensual design process. The workshop was held at the facilities of the academic partner, where the project manager, the business manager, the representative of the academic partner and the research team met. The workshop was animated by the main researcher, who gave the instructions and facilitated the activity. It was observed by two fellow researchers, who collected comments, appreciations, and interactions between the design team members. The development of the workshop began with the presentation of the results obtained in the individual interviews (Table 6-2). Based on it, the team members were asked to complete the following tasks:

- Discuss the presented design stages, their sequence and their names.
- Make agreements on their names, and elements (actors, inputs, outputs)
- Add or delete stages if necessary. Add or delete other elements if necessary.
- By each stage: What is decided? Is the decision process collective or individual? What are the challenges and criteria?
- By each stage: What are the IDOs along the process (IDO are concrete objects that are generated during the design process such as sketch, product sheet, sales pitch, industrial drawing, prototype, etc.)?

Table 6-2 Summary of the different views of the product design system according to the design team members (Business development manager Project manager Academical partner)

	Stage 1	Stage 2	Stage 3	Stage 4
Process Stages	Market observation Opportunity identification	Sharing customer needs in the team	Idea generation Feasibility of solutions	Validation of the solution Validation of the solution
Actors	-Project Manager -Business development manager -Final consumer -Customers -Trade or academic exhibitions -Producers of final cosmetic products -Business development manager -Enterprise Network	-Business development manager -Distribution partners network	-Project Manager -Business development manager -Academic partner -Sales assistants -Business development manager -Project Manager -Academic partner	-Academic partner -Project Manager -Academic partner -Project Manager
Input	-International exhibitions (commercial and academic) -Network of suppliers -Innovations of other companies and of universities -Regulations - Published reports by market research associations (trends and needs)	-Formulation or industrialization problem	-No used methods or resources -Expertise -Natural and regulated ingredients (INCI)	-Laboratory -Regulations -Key Ingredient -Deep documentary research
Outputs/ Result	-Market trends -Project mode: production or distribution -Potential idea -Needs to be satisfied (price & functional properties) -Market research	-Compiled information to satisfy the largest number of customers	-Technical feasibility report	-Solution to be validated -Potential key ingredient

	Stage 5	Stage 6	Stage 7	Stage 8
Process Stages	Sourcing of materials Sourcing of materials	Formulation: distribution mode Laboratory services Laboratory tests	Search for expertise	Processing of raw materials
Actors	-Project Manager -Academic partner -Raw materials Producers (Trusted partners) -Corporate network -Raw materials Transformers -Business development manager -Project manager	-Academic partner -Academic partner -Project Manager -Academic partner	-Academic partner -Project Manager	-Production plant
Input	-Market trends -Values from the parent company: Philosophy of the organization, traditional Chinese medicine, ethical work, responsible sourcing, etc. -Business process and financial research results -Target product specifications and properties -Technical recommendations	-Key Ingredients and extracts -Specifications and ingredients -Knowledge -Expertise -key ingredients -Preliminary literature search	-Technical Problem -Technical question -Knowledge - Expertise	-Search for financial and other resources -Acceptable Project maturity
Outputs/ Result	-Evaluation results and selection of potential producers -Commercial and technical study	-Results of test in cosmetic matrices -Efficacy and Performance Test -Performance characterization -Demonstrative formulas (prototypes) -Enhancing the value of ingredients -Ingredient validation	-Proposed solution (Formulation or premix)	

	Stage 9	Stage 10	Stage 11
Process Stages	Production mode formulation Formulation	Industrial production Scaling up to industrial scale	Communication
Actors	- Academic partner - Subcontracted laboratory -Academic partner -Academic partner (Statistician)	-Project Manager -Production plant (Independent actor, he is not a part of the design team) -Production plant -Project manager	-Graphic and web designers
Input	-Roadmap of steps to be done -Ingredients	-New design project	
Outputs/ Result	-Toxicological test -Regulations -Clinical efficacy -Sensory tests -Ingredient development -Support for scale-up	-Technical decisions -Resolution of scale issues related to product stability.	-Product technical brochure

Figure 6-2 shows the members of the design team and the white board on which they compared the design stages

Figure 6-2 Development of the formalization workshop with team members

The result is a formalized map of the design process, as shown in Figure 6-3 (the outcome of that day) and Table 6-3 (the digitalized result). The formalization workshop allowed the team members to determine by consensus the stages of the design process, resources needed, expected results, IDO, as well as identifying the most important decision at each stage.

During the formalization exercise it was noted that the team members appreciated the workshop significantly, because it allowed them to discuss their design process, which was not formally defined. They also shared between them details about their tasks, responsibilities, and expectations at each stage.

Figure 6-3 Outcome of the design process formalization workshop

Table 6-3 Map of the unified design process

	Stage 1	Stage 2	Stage 3
Process Stages	Market observation and opportunity identification (Permanent secondary activity)	Idea generation and solution evaluation	Solution validation
Actors	-Business development manager -Project manager -Academic partner		
Input	-Information from the sources: *International and academic trade exhibitions * Distribution network/Global organization *Market research reports *Facilitators/end users *Innovation of competitors *Regulatory information *Suppliers	-Available resources (including factory capacity)	-Laboratory tests and methods -Regulations -Candidate ingredients -Deep documentary research -Expertise
Outputs/ Result	-Potential Idea -Candidate ingredients -Market research / Market trends -Mode of operation: Production or distribution	-Technical feasibility report	-Applications of the ingredient
IDO	-Samples -Weekly meeting/ Report	-Weekly report (ppt) -Monthly "Academic partner"/Enterprise meeting -Specifications	
Decision	Mode of operation: Production or distribution (if it is more convenient to design a product and produce it, this design process continues, in the other case, this design process does not proceed, and a different planning should be made for product acquisition and distribution).		

	Stage 3	Stage 4	Stage 5	Stage 6
Process Stages	Formulation / Premix	Negotiation with the production plant	Production and transfer to the industrial scale	Communications and presentations plans
Actors	-Business development manager -Project manager -Academic partner (Statistician)	-Business development manager -Project manager -Production plant manager -Enterprise Director	-Project Manager Production plant Manager	-Graphic artists and designers -Business development manager -Project manager
Input	-Selected ingredient or extract to be formulated -Product specifications -Expertise -Problem or technical question to be solved in the formulation -Roadmap of steps to do	-Prototype -Developed idea -Technical reports of the academic partner	-Production project	-Academic partner and external laboratory results (additional tests)
Outputs/ Result	-Formulation development -Prototype formulas generation -Cosmetic matrix testing -Performance, efficacy, and sensory testing of prototypes	-Guide plans	-Technical decisions about industrial scale problems	-Product brochure -Product presentation (to customers and in commercial events) -Prototype
IDO	-Annual report -Prototypes -Laboratory notebook		-Production planning documentation	-Product brochure -Product presentation -Prototype
Decision	-Go or no go -Negotiation with the production plant	-Go or no-go to the production	-If a stable production is achieved, it is decided to go to the market	

6.2.2 Organization description development

This is a process that does not include the active participation of the design team members but is fed with the information collected in the preceding activities. Table 6-4 shows the organization's profile. It was done as explained in section 5.1.2.

Table 6-4 Case study organization profile

	Strongly ...	Disagree	Neutral	Agree	Strongly agree	Evaluation comments
	1	2	3	4	5	
Customer segments			x			The design team acquires knowledge about their customers from usage trends and consumer reports. There is not a specific task in the design process aimed at establishing the market segment of each product.
Value Propositions		x				The company has a clear value proposition in terms of the valorization of ingredients of Asiatic and natural origin. However, the company value philosophy is not the guide to all design decisions during the entire design process
Channels		x				There is a strong network of partners and collaborators who acts as source of information. However, during the development of the design project the channels of communication with direct consumer are limited. In this case, communication is always indirect and only happens at the beginning the of design projects.
Customer Relationship		x				The analysis of needs is indirect. There is not a strategic communication with the customers. During the formulation of the product there is little interaction with the consumer of the ingredient (cosmetic manufacturing companies and/or final consumer).
Revenue Stream			x			The organization has a clear strategy to collect financial resources. However, it was not mentioned as a decision criterion by the members of the design team in the formalization workshop.
Key Resources				x		During the development of the design project, the team has a clear knowledge about the resources available at each stage (financial, technological, human, among others).

Key activities	x					Before the workshop, each design member had his own vision of the design process. At the unification workshop, the establishment of agreements was neither evident nor natural, an important effort was invested to define key activities of the design process.
Key partners					x	The company's product design process recognizes and utilizes its extensive network of partners and contacts. At early design stages that network is a crucial source of information, greatly influencing the result.
Cost Structure			x			This element does not represent a major constraint to product development, nor is it widely discussed by team members

Key points

As a result of the exchange among the team members and their discussion during the workshop, some elements to be improve in their design process were identified. They are key points to be analyzed and worked on. They are shown in Table 6-5.

Table 6-5 Key points identified in the design stages

Design stage	Key points
Market observation and opportunity identification (Permanent secondary activity)	-No direct contact with the end user, and hardly any contact with the direct customer (cosmetic producers). -Lack of marketing staff to look for new customers -The network of customers is recent (as the design team), which requires a lot of attention from one person.
Idea generation and solution evaluation	-Innovation is constrained by regulations, and market capacity -Constraints on natural design and certification are new.
Solution validation	-No involvement of customers/users in the validation of the potential idea
Formulation / Premix	-No involvement of customers/users in the validation of the formulated product - No exit a specific step for final prototype validation
Negotiation with the factory	-The plant seems quite reluctant to work on new products in the cosmetics area and there is a lack of expertise in this area. - There is no effective communication between the production site and the formulator team
Production and transposition to industrial scale	-There are no clear guidelines for industrial accompaniment during the scaling process.
Communications and presentations plans	-The team does not have especial comments for this stage

6.2.3 Knowledge base interaction module

For the calculation of the score of the statements in the knowledge base, the organization profile and the key points are used as input. First, based on the company profile and applying Equation 5-2 Calculation *of the organization improvement vector*. It is presented in Table 6-6.

Table 6-6 Case study Organization improvement vector

By organizational context	Ideal value vector	Organization profile	Organization improvement vector
Customer segments	5	3	2
Value Propositions	5	2	3
Channels	5	2	3
Customer Relationship	5	2	3
Revenue Stream	5	3	2
Key Resources	5	4	1
Key activities	5	1	4
Key partners	5	5	0
Cost Structure	5	3	2

Then, the organization improvement vector is used to calculate the score of each statement as explained in section 5.2.1. The results are summarized in Table 6-7. Statements' scores range from 0 to 18, with a high-density distribution at intermediate scores.

Table 6-7 Case study statement score

Score	Statement identification number
18	4
12	60
10	86
9	21,23,43,36
8	1,44,70,95,96,32,40,42,68,100,101,102
7	8,49,30,51,52,79,74,75,82,93,94,108
6	6,22
5	12,34,5,11,20,24,41,103
4	18,29,58,83,14,13,35,50,85,16,15,26,27,33,37,39,45,46,47,53,54,55,56,57,59,61,64,65 ,66,67,72,76,77,78,79,80,81,84,87,89,90,97,98,106,107,109,111
3	2,7,10,19,25,31,62,69,91,92,99,104
1	9,28,48,71,105
0	17,3,38,63,88,110

Table 6-8 presents the results of this process. Here, the statements obtained by matching the knowledge base with the organization's profile and the key points are shown. At this stage, the statements are named as recommendations and are shown in the restitution module to the design team for their application.

Once the recommendations are filtered and ranked, those with the highest scores are proposed to the company for prioritization. For the case study, the entire list of recommendations was reviewed (for each design stage) but only the first 5 or 6 were selected, not all recommendations are proposed as this requires a significant investment of time for the design team analysis. Most appropriate statements for the company are subsequently identified by the screening process as explained in section 5.2.2. Only those statements related to design stages where there are concerns (key points) are selected.

As the filtering process progresses through the design stages, some of the recommendations may be in the preceding lists, special care is taken to avoid repeating them in those proposed to the design team.

Table 6-8 Case study recommendations presented by design stage

Market observation and opportunity identification (Permanent secondary activity)	**R1.** Clearly define and communicate your objectives in terms of costs and target audiences. Take into account your constraints in terms of production capacity and third-party contracts. **R2.** Study market trends based on the local environment and the global context. **R3.** Use techniques such as competitor benchmarking for customer needs analysis. **R4.** Evaluate projects that diversify markets. **R5.** Adapt formulations to the local costumer without losing the degree of originality. **R6.** Clearly choose your direction for the new product design. For example, choose between a new product innovation approach or an existing product imitation/adaptation approach.
Idea generation and solution evaluation	**R7.** Always make direct contact with the costumer **R8.** Base the formula proposal on the availability of raw materials and your possibilities of transformation processes **R9.** The information needed to decide must be clear: costumer needs, economic constraints, technical feasibility, product stability, production process, claims, and safety. **R10.** Keep in mind that design today is customer-centric. **R11.** Address the challenge of understanding the costumer and transforming their needs into technical needs

Solution validation	**R12.** Design approach is usually dictated by the available technology. **R13.** Allow the project manager to be the bridge between the different areas of the organization such as R&D, production site, suppliers, among others. **R14.** Manage logistical and inventory risks at the earliest stages. **R15.** Involve the pilot plant and production plant managers in the prototype launch and production planning. **R16.** Find allies in contractors, suppliers and distributors. **R17.** Validate your product conceptualization and ingredient selection with prototypes.
Formulation / Premix	**R18.** Take into account the user for efficacy or clinical tests, also in some sensory tests. **R19.** Base your new designs on the experience of the organization's previous projects. **R20.** Use user trials to adjust formulations **R21.** Offer product alternatives based on the local context of your costumers. **R22.** Consider elements of purchasing, warehousing, tracking codes, quality control, local delays, to scale up to commercial. **R23.** Generate quick prototypes to test with users, even if the formulation is not final
Negotiation with the factory	**R24.** Simultaneously adapt your design process to regulatory updates **R25.** Consider regulatory approval times and stability testing times in each project. **R26.** Use the industry ecosystem to gather information, testing and verification of quality. **R27.** Observe the impact of regulatory restrictions
Production and transposition to industrial scale	**R28.** Work with third party contractors when scaling up production at the production plant; maintain quality controls.

6.2.4 Restitution module

The restitution is conducted in the second workshop called, the recommendations workshop. From this workshop, the team members can identify concrete actions to align their design process with their strategy and business model and to solve key point issues. The recommendations that the company could implement is the base for the modification of their own chemical product design methodology. In the restitution workshop, team members evaluate the relevance and applicability of the recommendations in relation to the proposed scenarios of value creation.

Recommendations workshop

The recommendations workshop was conducted online using the online tools Mural and Microsoft Teams tools. It had the participation of the same team members of the first workshop, and it was carried out as follows:

Firstly, the results of the first workshop were presented to the design team, which included the company profile (Table 6-4), the identified key points (Table 6-5) and the recommendations extracted from the knowledge base (Table 6-8). Secondly, the participants were asked to select the value creation criteria for the evaluation of the recommendations. They were asked to propose them according to the company strategy for future them design projects.

Considering this, the team decided to work on the following three scenarios/value generation criteria: 1) How to be closer to the customers? 2) How to be more eco-responsible? 3) How to be more “digital” and have a better knowledge management?
Thirdly, the recommendations were discussed and evaluated by the design team based on its ability to generate value and its feasibility within the company. According to the results of this discussion, the team members placed each recommendation for each value generation criteria in a figure as the one presented in section 5.3. The results of the three evaluated scenarios are presented in Figure 6-4, Figure 6-5, and Figure 6-6.

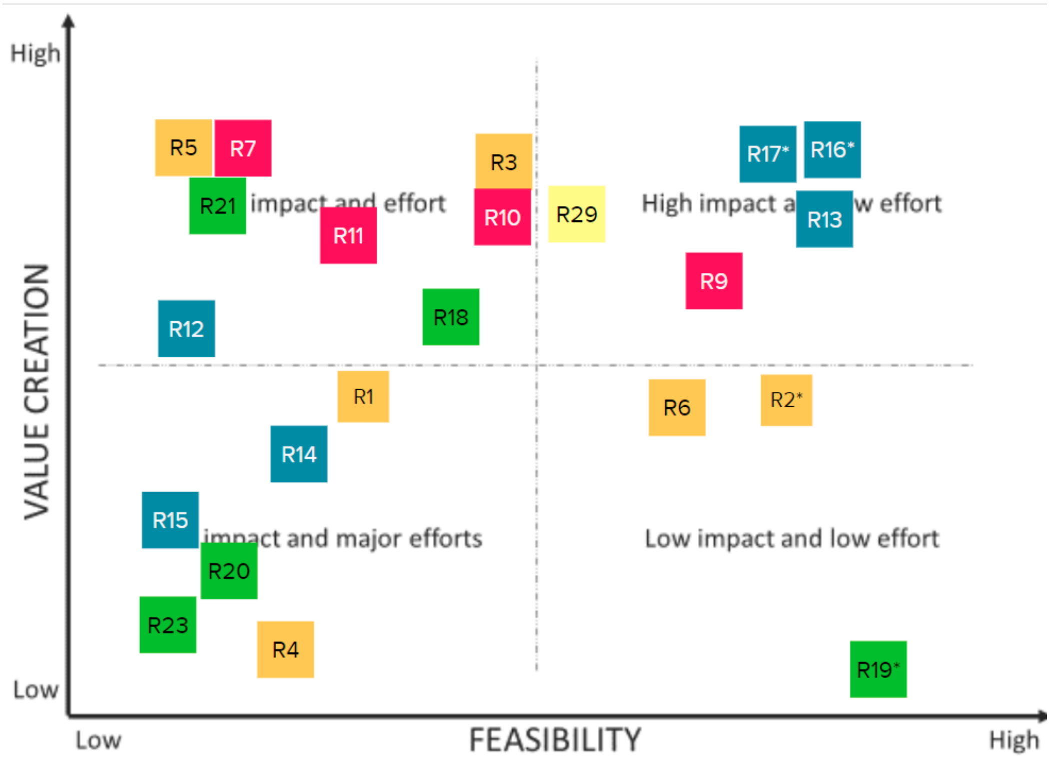

Figure 6-4 Prioritization of recommendations according to Criteria 1 How to be closer to the customers?

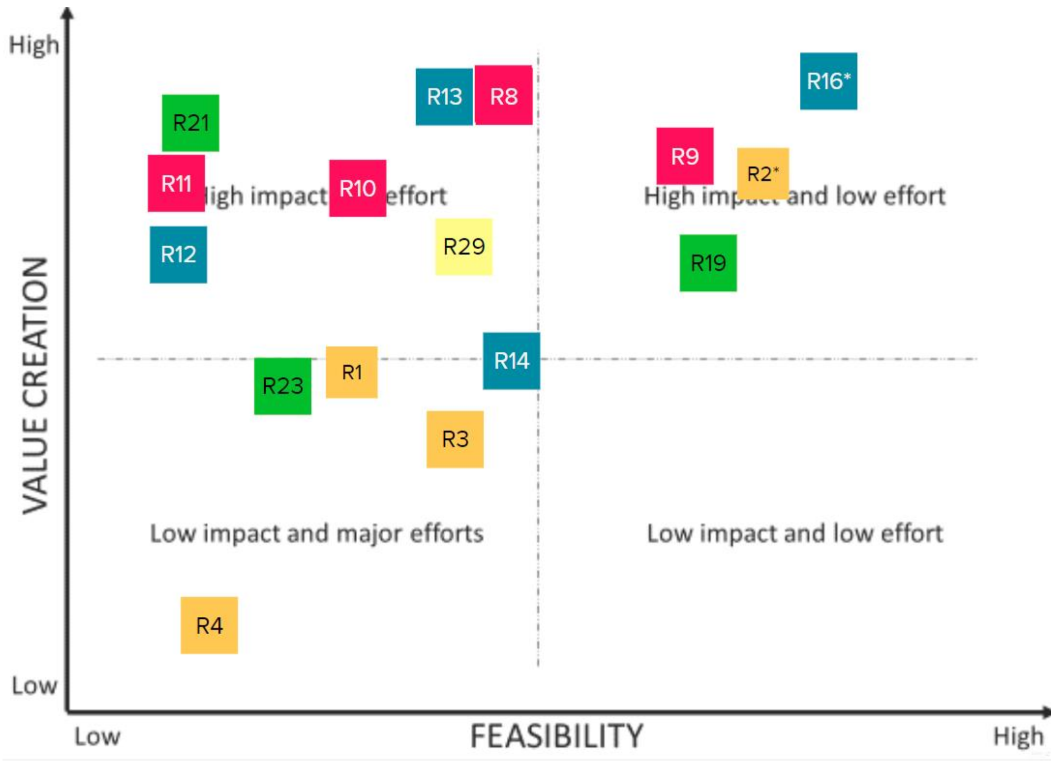

Figure 6-5 Prioritization of recommendations according to Criteria 2 How to be more eco-responsible?

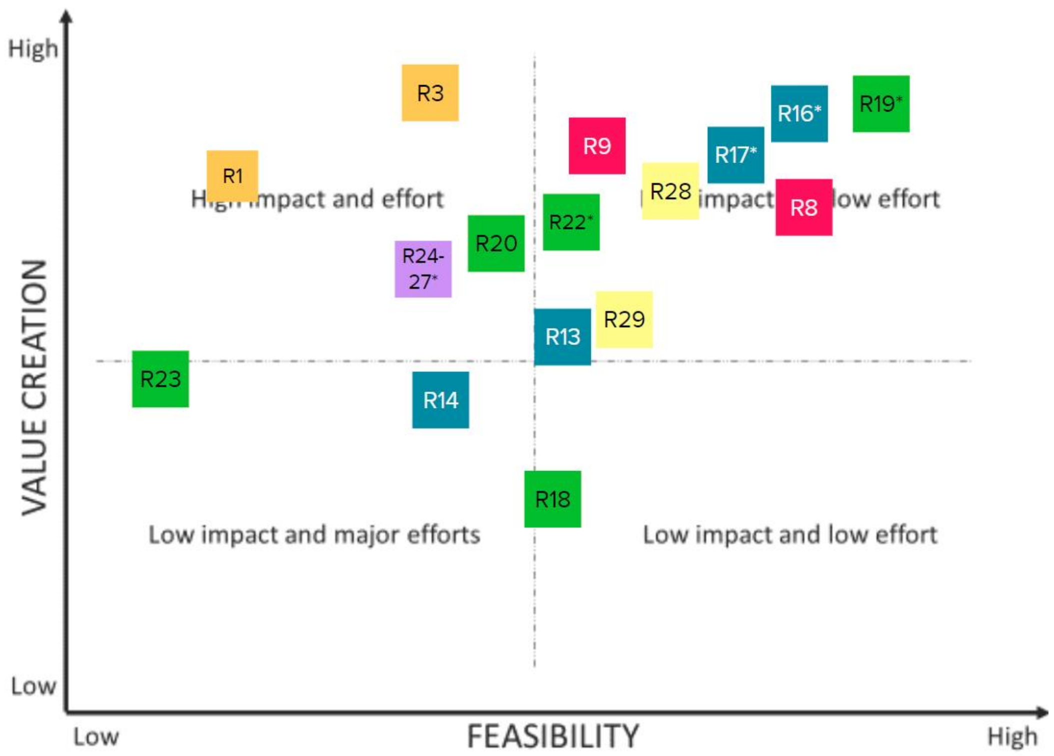

Figure 6-6 Prioritization of recommendations according to Criteria 3 How to be more “digital” and have a better knowledge management?

The application of the tool in the design methodology of the company, generated the following concrete results:

- It has been established that there are different design processes for the products that are formulated and for the products are distributed, they are two different processes for the design team that involve different efforts, here only the design process where the products are formulated was presented.
- The design team members agreed on a representation of the design process for the products formulated for their team. This agreement is important because it allows communication among them through vocabulary and common elements. Intermediate design objects make it possible to follow the evolution of the design process. In the same way, the identification of other actors who also participate in the design process helps to establish in advance possible bottlenecks to avoid in order to act quickly on them.
- The company profile shows its strengths and possible areas for improvement. It is highlighted as strengths the flexibility of the design process and the wide network of resources and connections. Possible areas for improvement are the strengthening of the relationship with its customers/consumers and their possible participation in the design process. Also, understanding the needs of end users (who are not direct customers, but are of great interest to their direct customers) could lead to the proposal of new innovative products.
- The workshops allowed the design team to communicate on topics that are not normally discussed on a day-to-day basis, but are fundamental to design, such as modeling the design process and company strategy. This is especially new information for the academic partner, who now has more tools to understand the decision criteria of the design process in order to propose technical solutions capable of meeting the company's objectives.

According to the ranking made by design team members, the applicable recommendations in all 3 scenarios that have a high potential to generate value and easily affordable are the following:

R8. Base the formula proposal on the availability of raw materials and the possibilities of the transformation process

R13. Allow the project manager to be the bridge between the different areas of the organization such as R&D, production site, suppliers, among others.
R19. Base your new designs on the experience of the organization's previous projects.
R28. Work with third party contractors when scaling up production at the factory; maintain quality controls.

The company must decide whether and how to implement some of the recommendations. Recommendations must be translated into concreate actions to modify the actual design process. For example, the recommendation R19, which states that new projects should be based on the company's experience, implies that the company applies knowledge and information management tools and methods. Since the design team was actively involved in understanding and ranking the recommendations, there is a basic agreement that should facilitate the interpretation and implementation of the recommendation in the design process.

6.3 Experience Feedback

Once the activities specific to the application of the tool were completed, participants were asked about the relevance of the tool in their design process, the applicability of the recommendations, and the quality of the tool in general terms. Based on this discussion, the following elements that constitute the feedback were identified:

- An important recognition is given to the activity of explicitly formalizing the design process. As expressed by one of the participants "Reflecting on the design process itself highlights the most frequent bottlenecks and allows for internal improvements."
- The tool allows to identify points to improve in the design process starting. This happens during the entire evaluation process, from the moment of the interviews until the formalization and recommendations workshop. This is attributed by the participants to the fact that those moments gave them a space for reflection.
- According to the participants, the impact of the application of recommendations in their product design methodology could be reflected in the medium term (months) and long term (years).
- The improvement actions emerging from the recommendations are a useful input for the generation of new strategies in the company's product design process. for example, this conclusion reached by one of the participants after

evaluating the recommendations “choosing the right direction for a new product between an innovation approach and copying an existing product. Also, the reminder that the design of a product is, nowadays, centered on the consumer”

Additionally, a questionnaire was implemented to know the opinion of the participants. (Supplementary material in Appendix C). The participants made the following comments:

- In general, the objectives of the tool and of all meetings between the design team and the research team were clear and comprehensible. The workload was appropriate for the result obtained. The pedagogical content of the discussions was also appreciated.
- some of the recommendations do not necessarily have to be evaluated on all the value creation criteria, the time of the workshops can be optimized by making a pre-evaluation of the recommendations
- Some of the company's particular key points are not covered by the recommendations.

6.4 Chapter conclusions

The aim of this chapter was to apply the product design methodologies support tool to a real case of cosmetic product design and development: the application is based on a qualitative validation method: the case study. The company was the subject of interviews and workshops, with the aim of, on the one hand, operationally testing the tool (does it work properly?) and, on the other hand, to check the relevance of the proposed results, by confronting them with the point of view of the members of the company's design team. Thus, the implementation of the tool included several phases: a preparation phase, an interview phase, an analysis phase (evaluation of the company), a recommendations and prioritization phase, and finally a discussion phase on the relevance of the tool and its results. In general, the comments on this tool are encouraging. The overall vision of the formalization strategy plus recommendations has raised the curiosity of the company's design team members, and the fact of being able to choose their own improvement scenario, or even to compare several, promoted a discussion of perspectives for new product design methodologies.

In addition, this tool seems relevant for cosmetic ingredient formulation companies, however, there are some limitations. Some recommendations lacked relevance, given their current application in the company's internal processes.

Thus, the tool, in its current state of development, is limited in managing certain specificities linked to the current state of the company's design process. The main prospect for improvement is therefore to make it more flexible and adaptable, in order to propose an even more relevant assessment and recommendations that make sense for each of the companies assessed. Consequently, the tool is susceptible to improvement. However, it can be considered a promising first version in view of the feedback from the company design team. Initially conceived as a decision-support tool, which allows to act directly on companies to improve their product design process, it allows to propose to companies levers of action. However, it does not yet reach the construction of an operational action plan for its implementation to develop its facet as a decision support tool. The tool also acts as an educational tool for the design team by encouraging the team to ask questions about the organization of their company and their design process, bringing to light elements they had not considered or formalizing their own organizations. One improvement perspective is the vocabulary used to describe the different design stages. The experimentation shows that people in the design process give different names to the same stage. Thus, some clear generic terms and explanation may help to get a more rapid consensus about the current process.

7 Conclusions and future work

The thesis defended in this document considers the design and development of chemical products as a system highly dependent on its organizational context. Therefore, a comprehensive and detailed view of that system is proposed to enable design teams to understand the impact of their involvement and decisions along the design process.

This research proposes a systems analysis approach for the comprehension of the chemical design projects in organizations. Results of this analysis are subsequently exploited through the creation of a tool to support the management of the design process, encouraging organizations to use systems thinking for their product design methodologies improvements.

7.1 Contributions

This document provides several contributions linked to different scientific domains in the chemical product design problem:

Triggers for Chemical Product Design: A comprehensive theoretical basis was established to justify this work. A bibliometric analysis of the latest publications in the chemical product design field was made. Those publications were analyzed in three main axes: type of product, organizational context, and phases of the product design methodologies presented by the authors. Thanks to this analysis, the bases for the development of this research were established: first, it was found that the formulated products are an object of interest for most of the authors, because their design involves important scientific challenges, and due to their high added value. Second, product design methodologies lack an integrated approach that considers all stages of product design; especially the needs analysis is poorly understood. Finally, it was found that the context in which the design process takes place, i.e., the context of the organization, its limitations and possibilities are not considered when proposing design methodologies to a great extent.

Chemical product design in an organizational context: A product design system analysis methodology was proposed with two objectives 1) to describe the system that is created when organizations design chemical products and 2) to understand the needs of organizations to implement product design and development strategies. The analysis methodology was applied to eleven case studies with design experts of companies in different industrial sectors, all of them with experience in the design of formulated products and most of them in the cosmetic sectors. The analysis enabled the identification of actors, design stages, resources, and interconnections of elements in the analyzed design processes. In addition, several particularities of the product design systems were found: The design process is specific to the organization. The organizational environment provides constraints and facilitators that articulate the design team. Moreover, it is a system that extends beyond the organization's boundaries, considering key external stakeholders, such as suppliers and regulatory agents, among others. Notably, the needs of the users are the focal point of the product design. There is a lack of clarity among the actors involved in the design task, a situation that can generate complications for the design team.

Towards a knowledge base to support product design considering organizational context: Here, a knowledge base was created and developed in which knowledge shared by experts in chemical product design and development is presented in an organized and exploitable manner. For this contribution three steps were followed: information gathering, the creation of an analysis framework, and the extraction and characterization of recommendations. The resulting knowledge base is the foundation for the construction of an analysis tool of the design process in organizations. It contents recommendations that can be used for organizations to improve their design process. Additionally, the methodology used for the construction of the knowledge base is an approach that can be used by organizations to store and organize their implicit knowledge acquired through experience.

Construction of a tool to support the management of the chemical product design process The tool proposed here is the integration of the previous contributions. The tool seeks to support the design of chemical products in organizations. Understanding that design is a highly context-dependent process, the tool is based on a participatory method that allows the design team members to actively collaborate in the generation and the evaluation of recommendations for the improvement of the design process. The tool consists of three modules: the first, to understand the current state of the organization's design process using the system analysis approach described above; the second, to extract recommendations for improvement of the design process from the knowledge base; and the third, to evaluate the relevance of the recommendations considering value concepts of interest for the organization.

Application of the tool to a real case Using a case study, the tool proposed in this research was applied with the following objectives: 1) to test the operation of the tool, by establishing concrete protocols for interviews and workshops, and 2) to test the relevance of the proposed results against a real case and a real design team. The application allowed to verify the functioning of the tool. The tool allowed the design team to know and formalize their daily activities in a formal product design process. Moreover, the participatory approach used for the tool demonstrated its acceptability, adaptability, and relevance. Additionally, the recommendations generate several perspectives to improve their own product design processes in alignment with strategic value concepts for the company.

The above contributions respond to the objectives of this research, which aimed to integrate the system that is created in the organization when designing chemical products, creating and testing a tool that allows updating the methodologies of product design of the companies.

7.2 Perspectives

Keeping in mind the above, the opportunity is created to present some additional perspectives for the research and for the tool proposed in this document.

In-depth tool development. In this research, a case study was carried out with one company in France that produces cosmetic formulated ingredients. The results of the tested qualitative approach are promising and demonstrate its relevance. However, it seems necessary, in order to judge the relevance of the tool from a general point of view, to test this tool with a larger number of companies from different sectors of the cosmetic production chain and with variable characteristics in the design teams. Indeed, a quantitative validation would provide solidity to the tool. However, such study will have to consider the dynamic reality of the organizations and their processes.

Strengthen the characterization of the profile of the organization. The study can be complemented by considering the effect of the human dimension in the design process. In this study, this dimension was indirectly considered by characterizing those involved in the design in the form of activities and observable phenomena in the system mapping. The human dimension has not been fully integrated in our study, but it opens an interesting research perspective, for example, in the study of the profile of leaders within the members of the design team. Additionally, a maturity modeling approach can be useful for assessing the organization's profile, including different dimensions like human and technological, among others. The maturity assessment can be developed on a sequence of steps containing elements that describe the characteristics of the profile of the organization at a given level of development.

Maturity of the database. The proposition of recommendations based on the knowledge base is promising, even considering that at the time of the application of the tool, it was still young and had a relatively low participation of experts. A constant feeding of the knowledge base as well as an additional data processing could generate more adapted recommendations. Additionally, the integration of experts with other areas of knowledge is necessary to extend the current knowledge base to other areas of knowledge in product design and development such as marketing, software development, innovation, consumer psychology, among others.

Appendix A. Literature review sample.

Table A-1. Publication summary regarding chemical formulated products (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)

Ref.	*Product type*				*Design stages*					*Business approach*		*Sector*
	Com	*Mol*	*Dev*	*For*	*Nee*	*Tra*	*Alt*	*Sel*	*Pro*	*Stru*	*Stra*	
(Wibowo & Ng, 2001)				x	x	x	x	x				Cos.
(Wibowo & Ng, 2002)				x			x					Pha.
(Rähse & Hoffmann, 2002)				x	x			x		x		Un.
(Fung & Ng, 2003)				x	x		x	x				Pha.
(Rähse & Hoffmann, 2003)				x	x	x	x	x		x		Un.
(K. M. Ng, 2003)		x		x	x		x	x	x	x	x	Un.
(Meyer & Keurentjes, 2004)	x			x			x					Pol.
(Bernardo & Saraiva, 2004)				x			x	x				Cos.
(J. Abildskov & Kontogeorgis, 2004)	x			x			x					Pol.
(Hill, 2004)				x				x		x		Cos.
(K. M. Ng, 2004)				x	x		x	x	x			Un.
(K. M. Ng et al., 2005)				x	x		x	x		x		Un.
(Muro-Suñé et al., 2005)				x	x		x					Pha.
(Bernardo & Saraiva, 2005)				x	x		x					Cos.
(Yu et al., 2006)				x			x		x			Un.
(Perrot et al., 2006)				x		x						Food.
(Qian et al., 2006)				x			x	x	x			Un.

Ref.	*Product type*				*Design stages*					*Business approach*		*Sector*
	Com	*Mol*	*Dev*	*For*	*Nee*	*Tra*	*Alt*	*Sel*	*Pro*	*Stru*	*Stra*	
(Gong et al., 2006)				x	x		x	x				Food.
(M. J. Bagajewicz, 2007)				x				x	x	x		Pha.
(Feng et al., 2008)				x	x		x	x				Food.
(Costa et al., 2008)				x			x					Pha.
(Bongers & Almeida-Rivera, 2009)				x	x		x	x	x	x		Food.
(Conte et al., 2009b)				x			x		x			Cos.
(Yuen S. Cheng et al., 2009)				x	x		x	x		x		Cos.
(Conte et al., 2009a)		x		x			x	x	x			Ink.
(Smith & Ierapepritou, 2009)				x	x	x				x		Cos.
(Solvason et al., 2010)				x			x	x				Pha.
(Omidbakhsh, Elkamel, et al., 2010)				x	x		x	x				Hom.
(Omidbakhsh, Duever, et al., 2010)				x			x	x				Hom.
(Stelzer & Ulrich, 2010)				x			x		x			Ink.
(Yuen S. Cheng et al., 2010)				x		x				x		Pha.
(Wu et al., 2010)				x			x	x				Food.
(M. Bagajewicz et al., 2011)				x	x		x	x		x		Cos.
(Linehan et al., 2010)				x	x	x	x					Food.
(Frenkel, 2011)				x			x		x			Un.
(Conte, Gani, & Malik, 2011)				x			x	x				Cos.
(Jens Abildskov & O'Connell, 2011)				x			x	x				Ink.
(Conte, Gani, & Ng, 2011)				x			x	x				Cos.
(Cholakov, 2011)		x		x				x		x		Ink.
(Picchioni & Broekhuis, 2012)				x					x			Un.
(Conte et al., 2012)				x			x	x				Cos.
(J. Victoria Villeda et al., 2012)	x			x			x	x	x			Ink.

Ref.	Product type				Design stages					Business approach		Sector
	Com	*Mol*	*Dev*	*For*	*Nee*	*Tra*	*Alt*	*Sel*	*Pro*	*Stru*	*Stra*	
(J. Victoria Villeda et al., 2012)				x				x				Cos.
(Warrier, Sathyanarayana, Patil, et al., 2012)				x			x	x				Ink.
(Ariffin Kashinath et al., 2012)				x			x					Ink.
(Warrier, Sathyanarayana, Bazdar, et al., 2012)				x			x					Ink.
(Omidbakhsh et al., 2012)				x	x	x		x	x			Hom.
(Wassick et al., 2012)				x				x		x		Un.
(Martín & Martínez, 2013)				x	x		x	x	x			Hom.
(Samudra & Sahinidis, 2013)				x			x					Ink.
(Heintz, Belaud, & Gerbaud, 2014)				x	x		x	x		x	x	Ink.
(Heintz, Belaud, Pandya, et al., 2014)				x			x	x				Ink.
(Santos et al., 2014)				x			x	x				Ink.
(Santos et al., 2014)				x	x	x	x					Cos.
(L. Y. Ng et al., 2014)		x		x	x		x	x				Ink.
(Bergez-Lacoste et al., 2014)		x		x	x		x	x				Ink.
(Mattei et al., 2014)				x			x	x				Cos.
(Tomba et al., 2014)				x			x	x				Pha.
(Ewoldt, 2014)				x			x	x				Ink.
(C. K. H. Lee et al., 2014)				x	x		x	x		x		Cos.
(Yunus et al., 2014)	x			x	x	x						Ink.
(Pavurala & Achenie, 2014)				x			x	x				Pol.
(Bernardo & Saraiva, 2015)		x	x	x	x		x	x				Cos.
(Azmin et al., 2015)				x	x		x	x				Ink.
(J. J. Victoria Villeda et al., 2015)	x			x			x	x		x		Ink.
(Chong et al., 2015)				x			x	x				Ink.
(L. Y. Ng et al., 2015)	x			x	x		x	x				Ink.

Ref.	*Product type*				*Design stages*					*Business approach*		*Sector*
	Com	*Mol*	*Dev*	*For*	*Nee*	*Tra*	*Alt*	*Sel*	*Pro*	*Stru*	*Stra*	
(Martín & Martínez, 2015)				x			x	x	x			Hom.
(Abdul Rahim et al., 2015)				x	x		x	x		x	x	Pol.
(Fatoni et al., 2015)				x	x	x	x	x				Pol.
(Yuen Shan Cheng et al., 2016)				x	x	x	x	x		x		Food.
(Chong, Foo, et al., 2016)				x	x			x				Ink.
(Dahmen & Marquardt, 2016)				x			x	x				Ink.
(Austin, Samudra, et al., 2016)				x			x	x				Ink.
(Jonuzaj et al., 2016)		x		x			x	x				Ink.
(Tam et al., 2016)				x			x	x				Ink.
(Kiskini et al., 2016)		x		x			x	x	x			Food.
(Chong, Eljack, et al., 2016)				x			x	x				Ink.
(Fung et al., 2016)		x	x	x	x	x	x	x	x	x	x	Ink.
(Alvarez, 2017)				x	x		x	x		x		Un.
(Wan Qi et al., 2017)				x	x	x	x	x				Ink.
(Khor et al., 2017)				x			x	x				Ink.
(Frutiger et al., 2017)				x			x	x				Ink.
(Yang et al., 2017)				x				x				Pol.
(Jonuzaj & Adjiman, 2017)				x			x	x				Ink.
(Dahmen & Marquardt, 2017)				x			x	x				Ink.
(Holmes et al., 2017)		x		x	x		x	x				Un.
(L. Zhang et al., 2017)				x	x		x	x				Hom.
(Hada et al., 2017)				x			x	x				Pol.
(Kashinath et al., 2018)				x				x				Ink.
(Martín & Martínez, 2018)				x				x				Hom.
(Cignitti et al., 2018)	x	x		x			x	x				Ink.
(Serna et al., 2018)				x	x	x	x	x				Cos.
(L. Zhang, Kalakul, et al., 2018)				x	x		x	x				Ink.
(Derkyi et al., 2018)				x	x			x				Food.
(Y. C. Chan et al., 2018)				x	x		x	x		x		Food.

Ref.	*Product type*				*Design stages*					*Business approach*		*Sector*
	Com	*Mol*	*Dev*	*For*	*Nee*	*Tra*	*Alt*	*Sel*	*Pro*	*Stru*	*Stra*	
(L. Zhang, Mao, et al., 2018)				x			x	x				Cos.
(Kalakul et al., 2018)		x		x	x		x	x				Ink.
(Xiang Zhang et al., 2018)				x	x		x	x		x	x	Pol.
(Kontogeorgis et al., 2019)				x	x	x	x	x	x			Cos.
(Arrieta-Escobar et al., 2019)				x	x		x	x				Cos.
(Frutiger et al., 2019)				x			x	x				Ink.
(C. K. H. K. H. Lee, 2017)				x	x	x	x					Cos.
(Lai et al., 2019)				x	x		x	x	x	x	x	Ink.
(Rafeqah et al., 2019)				x				x				Ink.
(Jhamb et al., 2019)				x			x	x				Un.
(Liu et al., 2019)				x			x	x				Ink.
(Neoh et al., 2019)				x			x	x				Ink.
(X. Zhang et al., 2019)				x			x	x		x		Hom.
(Liang et al., 2019)				x			x	x				Pol.
(Xiang Zhang et al., 2019)				x	x	x	x	x	x			Food.
(Nelson et al., 2019)				x			x	x				Pol.
(Jonuzaj et al., 2019)				x			x	x				Ink.
(Torres et al., 2020)				x	x		x	x		x		Cos.
(Jhamb et al., 2020)				x			x	x				Ink.
(Cardona Jaramillo et al., 2020)				x			x	x				Un.
(König et al., 2020)		x		x			x	x	x			Ink.
(Marques et al., 2020)		x		x			x	x		x	x	Pha.
(Papadopoulos et al., 2020)		x		x			x	x				Ink.
(Chai et al., 2020)		x		x			x	x	x	x	x	Ink.
(K. C. Cheng et al., 2020)				x			x	x				Hom.
(Sunkle et al., 2020)				x				x				Cos.
(Raslan et al., 2020a)				x				x				Ink.
(Mushtaq et al., 2020)				x			x	x				Ink.
(Raslan et al., 2020b)				x				x				Cos.
(Taifouris et al., 2020b)				x			x	x		x		Ink.

Appendix B. Complete list of statements and its categorization

Table B-1 Statements that constitute the knowledge base

Number	**Statements**
1	Clearly choose your direction for the new product design, choose between a new product innovation approach or an existing product copy approach.
2	Align your design project goals with the geographic and demographic context of your organization.
3	If possible, ask about the formulation services offered by the suppliers of the raw materials they provide.
4	Clearly define and communicate your objectives in terms of costs and target audiences. Take into account your constraints in terms of production capacity and third-party contracts.
5	If your design process is based on an innovative approach, focus on meeting the needs of your users.
6	Validate your product conceptualization and ingredient selection with prototypes.
7	Use market trends as a guide for your design projects.
8	Base your new designs on the experience of the organization's previous projects.
9	Try to make maximum use of the help provided by the suppliers
10	Feed your design process with information from market trend analysis and strategic business objectives.
11	Establish initial contact with your suppliers to assess the feasibility of your product concepts. Don't forget the local context of your suppliers
12	Offer product alternatives based on the local context of your consumers.
13	Simultaneously adapt your design process to regulatory updates
14	Generate quick prototypes to test with users, even if the formulation is not final
15	Consider production capacity, packaging restrictions and logistics to move to a final formulation.
16	Work with third party contractors when scaling up production at the factory; maintain quality controls.
17	Find allies in contractors, suppliers and distributors.
18	Design approach is usually dictated by the available technology.
19	Establish if your design process is based on adding value to scientific developments
20	Have a clear understanding of the availability of resources when conducting market research.
21	Use techniques such as competitor benchmarking as input to customer needs analysis.

22	Establish stages of direct testing with users, in addition to satisfaction tests.
23	Evaluate projects that diversify markets.
24	Develop in parallel activities of market analysis, advertising, marketing, brand development and the search for potential customers.
25	Establish the different business models according to the target products and by-products.
26	Please note that regulatory limits vary depending on the type of ingredients and the type of product.
27	be clear and inform your product design team of your process for product design and development
28	be clear about your process for product design and development, let your product design team know the process
29	Allow the project manager to be the bridge between the different areas of the organization such as R&D, production site, suppliers, among others.
30	Exploit the process of product ideation, packaging, redesign, building the link between the commercial sector of the company and R&D
31	Study the opportunities that arise from the trends evidenced in market research.
32	Evaluate in the early stages of design: feasibility of concepts, commercialization, formulators and regulatory agencies involved, and technology available.
33	Encourage oversight and validation of product technical risks by formulators.
34	Consider elements of purchasing, warehousing, tracking codes, quality control, local delays, to scale up to commercial.
35	Consider regulatory approval times and stability testing times in each project.
36	Take into account the user for efficacy or clinical tests, also in some sensory tests.
37	Consider the bureaucratic tradeoffs within your organization in your design project.
38	Involve suppliers as early as possible in the design process
39	Always establish which processes can be done in-house and which ones need a third party
40	Do not only take into account technical requirements when making decisions, include sustainability elements throughout the design (suppliers, process, formula, packaging).
41	Consider the mission and vision of the organization as a guide in the process of designing a new product.
42	establish a differentiation strategy to your customers
43	Adapt formulations to the local consumer without losing the degree of originality.
44	Base the formula proposal on the availability of raw materials and the possibilities of the transformation process
45	use techniques such as design of experiments to adjust recipes or formulations
46	Keep in mind that the relationship with suppliers influences the new recipes/formulas.
47	Obtain information about synergies between ingredients from suppliers
48	The experience of formulators is important in predicting the behavior of ingredients.
49	Use user trials to adjust formulations

50	Use the industry ecosystem to gather information, testing and verification of quality.
51	Establish which innovation model will guide the product design; for example, "agile" or "user-centric".
52	consider the marketing strategy and the vision of the directives as a guide in the process.
53	Turn the technical area into a strategic partner of the marketing area.
54	Find the balance between marketing visions and technical proposals.
55	define whether the formulator plays an all-inclusive role or a technical role
56	Anticipate complexity by coordinating the different teams within the organization.
57	Consider the size and bureaucracy of the company, the flow of information may be affected.
58	Manage logistical and inventory risks at the earliest stages.
59	involves a global vision of the whole process in design
60	Always make direct contact with the consumer
61	Involve marketing, market research, purchasing, finance, suppliers, inventories in the formulation process.
62	Establish what the company's strategic objective is and see how it affects the design process.
63	Decide whether or not the suppliers can be considered as design partners.
64	Establish clear objectives and product claims early on to assess legal feasibility with regulators.
65	Use technical tools such as design of experiments
66	Consider a policy of "In the laboratory it is better to fail fast".
67	Contrast the proposed design concept with the interests of the organization.
68	If your business strategy is consumer-oriented, design decisions should be less bureaucratic.
69	avoid personal biases of the formulator by putting him/her in contact with the consumer
70	The information needed to make a decision must be clear: consumer needs, economic constraints, technical feasibility and product stability, production process, claims, safety.
71	consider time as a resource for decision making
72	Tailor your process to the skills of the design team.
73	Be clear about your business and strategic model
74	Integrate organizational culture and business model into your design
75	Define which design strategy to follow, e.g., "mass consumption" or "direct sale".
76	Base new product design on marketing trends and market studies
77	Let the research and development groups become the leaders of the project.
78	Articulated your projects with the Research and Development team for decision making
79	Establish the relevance of the project between Marketing and R&D.
80	At the prefeasibility stage, all sectors of the company may be present, including the president of the company.
81	review the feasibility of the project based on the company's resources and led by Research and Development.

82	Establish validation points with the consumer at each stage of the design process; concept, prototype, advertising, performance.
83	Involve the pilot plant and production plant managers in the prototype launch and production planning.
84	Allow suppliers to become an important source of information for prototype and concept development.
85	Observe the impact of regulatory restrictions
86	Study market trends based on the local environment and the global context.
87	Enable articulations and communications between teams with clear information on costs, concepts; claims.
88	Consider suppliers as a basis for the formulation
89	Allows the formulator to articulate the logistics and inventory teams
90	allow the formulator to be the link between consumer and planning and production.
91	Establish an organizational structure that allows decisions and ideas to be made by more than just one person
92	Please note that each company dictates its own operational approach to product design.
93	Every product design starts with trends
94	Depending on the organizational strategy, trends can be followed or created.
95	Keep in mind that design today is consumer centric.
96	Address the challenge of understanding the consumer and transforming their needs into technical needs
97	Ensure that the formulator knows and is aware of the user and the marketing language.
98	The technical know-how is acquired through experience
99	Understand that trends are born, grow and die.
100	Capturing trends and insights is possible in all types of companies.
101	Define your design strategy, satisfy unsatisfied needs or propose disruptive products.
102	Understand the user's pain.
103	Monitor trends in the formulations generated by social media influencers
104	Find product insights not only in novel formulations, but also use innovation in other areas such as product communication.
105	Design according to the realities and the context; costs, production plant...
106	Control the appearance of hierarchies in decision making
107	Begin the design process with as much clarity as possible, a benefit is given to the project.
108	Inform the whole team of the project objectives
109	allow the formulator to become a negotiator in the negotiation process.
110	Understand that suppliers are key partners for the design, they are the ones who develop the technology.
111	Avoid delays or damage to resources due to complicated decisions
112	Involve the entire design team in the early design stages.
113	Let the formulating team have input throughout the design process.
114	Be aware of constraints given by access to resources, materials and technology
115	Be clear about the objectives of the project and the regulatory constraints you will face

116	Involve the user as quickly as possible, validate in different stages of the design.
117	Know the structure and process of the design team.
118	Find key partners in suppliers and service providers.
119	Consider the needs that a new product generates for the logistics, warehousing and purchasing areas.
120	Share timing, objectives, and resources available for the project from the beginning
121	Allow the technical area to have a voice when final decisions are made.
122	Solve problems on the spot, get representatives from the most relevant areas to discuss
123	Consult regulatory issues before making radical changes in formulations
124	Save, organize, and use experience from previous projects
125	Anticipate product life after manufacture, reflect on how this affects the user
126	Always ensure the safety of your product, use different sources of information, in addition to testing.
127	Set key tasks for each area of the organization involved, turn them into experts
128	Recognize and give importance to the technical side of the design.
129	Manage the knowledge of experience acquired in previous developments.
130	Establish objective tests that allow you to quickly validate prototypes
131	Build consensus among the areas of the organization that are affected by a new product.
132	Develop product scale-up at the same time as formulation
133	Document the design process
134	Establish sustainability, safety, and resource use targets

Table B-2 Statements that constitute the knowledge base

Number	Preliminary trend studies	User needs identification	Organizational needs	Product conceptualization	Supply chain logistics	Technical feasibility	Product technical concept	R&D Development	Formulation process	Packaging engineering	Pre-prototype	Technical validation	Prototype	User Validation	Legal Validation	Scaling-up	Final approval	Process standardization	Project closure	Accompaniment to production	Directives	Marketing	Supply chain	Purchasing	Sales	Formulator	Production	Logistic	User/client	Project chef	Supplier	Legal team	External laboratories	Contract manufacturers	Academic partner	Regulatory entities	Industry ecosystem	Social Media Influencers	Customer segments	Value Propositions	Channels	Customer Relationship	Revenue Stream	Key Resources	Key activities	Key partners	Cost Structure
1	1	1																			1	1																		1				1	1		
2	1	1		1		1																1	1	1	1														1					1		1	
3				1		1	1		1		1												1			1					1															1	
4	1	1										1		1		1				1	1	1	1		1	1	1													1	1	1	1	1	1	1	1
5	1	1	1											1								1							1										1	1							
6							1		1		1		1									1				1	1		1										1						1		
7	1	1																				1				1														1							
8									1												1	1								1										1					1		
9				1		1	1		1																	1					1													1			
10	1	1	1																		1	1							1	1										1							
11	1			1		1	1		1													1				1				1	1													1	1	1	
12		1							1													1								1									1	1							
13												1			1			1	1							1						1													1		
14									1		1		1	1								1				1			1	1															1		
15									1							1		1	1							1	1			1															1		
16																1		1		1						1	1			1															1	1	
17					1	1										1		1			1	1				1					1			1												1	

18						1	1		1			1				1		1								1	1			1										1				1			
19	1			1		1																				1									1					1						1	
20	1	1	1	1																	1		1	1		1	1																	1	1		
21	1	1	1	1																	1	1				1													1	1					1		
22		1												1								1				1			1											1		1					
23	1	1	1																		1	1								1									1	1					1		
24	1	1	1	1																	1	1																	1	1							
25	1	1	1	1					1												1	1				1														1							
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27																					1	1																							1		
28																					1	1				1				1														1			
29					1	1		1	1																																				1		
30			1					1		1											1	1				1														1					1		
31	1	1	1	1																	1	1				1														1							
32	1	1	1	1					1						1							1				1						1				1				1				1	1	1	
33							1		1			1						1								1	1			1															1		
34					1				1	1								1	1						1		1			1														1	1	1	
35												1			1											1							1	1											1		
36		1							1			1	1	1												1				1	1		1						1			1			1		
37				1		1						1			1		1				1	1								1															1		
38					1				1														1			1					1															1	
39																																													1		
40	1			1		1						1					1				1	1	1	1	1	1	1													1				1	1	1	
41	1	1	1	1																	1	1				1													1	1							
42	1	1	1	1																	1	1				1													1	1		1					
43	1	1	1	1																	1	1				1			1										1	1					1		
44				1	1		1		1									1																						1				1	1	1	

45								1																	1									1										1		
46			1	1		1		1														1			1					1														1	1	
47			1	1		1		1														1			1					1														1	1	
48			1					1																	1																		1			
49								1				1	1			1									1			1	1												1			1		
50											1		1	1		1									1				1							1								1	1	
51																				1									1										1					1		
52	1	1	1																	1	1																		1					1		
53	1	1				1		1			1										1				1				1															1		
54	1	1				1		1			1										1				1																			1		
55			1			1		1			1														1																			1		
56																									1				1															1		
57																													1															1		
58				1	1				1							1	1					1	1							1														1		
59																													1															1		
60		1		1						1		1	1			1					1				1			1	1									1		1	1			1		
61	1	1			1			1													1	1	1		1					1														1		
62																				1	1																		1							
63					1			1														1			1					1															1	
64						1					1			1											1				1		1				1									1		
65								1																	1																			1		
66								1																	1																			1		
67						1										1				1																								1		
68		1											1							1								1										1	1		1					
69		1						1					1												1			1													1					
70			1		1						1			1		1				1	1	1	1	1	1	1	1		1		1	1										1		1		1
71																1													1														1			

72									1												1									1															1		
73																					1									1										1					1		
74																					1									1										1					1		
75																					1									1										1					1		
76	1			1																		1								1															1		
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Appendix C. Supplementary material prepared for work with companies.

Individual interview protocol for team members

Welcome and et presentation - Max 5 min	
Project and interview presentation - Max 5 min	
1: Knowing the interviewee	
Question	**Objective**
Profile	Determine the interviewee's profile, experience, area of expertise, professional career, position in the company.
Enterprise profile	Size of the company, how the company is organized, where they are present, what is their value proposition, do they know the mission or vision.
2: How product design is carried out	
For you, how does the design of a new product usually start?	Ask the interviewee for an overview of the product design process. Ask for the description of the stages, the actors, the key elements for the product design.
What kind of decisions do you usually face within the project?	Inquire about the type of information used to make decisions, at what point in the design project. It should also be established if there are hierarchies at the moment of decision making.
At what point do you consult your colleagues, users or third parties throughout the project?	Understand how the type of information that allows the interviewee to make easy decisions, at what point the different actors of the design teams should be coordinated

Formalization Workshop Protocol

Activity	Duration (min)	Objectif
Reception	**05:00**	Reception of participants. Personal introductions of the workshop participants and the facilitators will be made. Workspace allocation
Introduction	**05:00**	Opening of the activity. Presentation of facilitators and the role of each one: Presentation of the project and the workshop.
Feedback and discussion	**10:00**	Give feedback of the interview process and results.
Guidelines Part 1	**05:00**	Explain the objective of the first part of the workshop, explain the canvases that will be used and how they are expected to be filled out
Draw the current process	**30:00**	Participants should draw their current design process according to the workshop guidelines. To have a pre-filled board with the compendium of the design processes of the interviewees. Have movable cards to complete or modify the process and a blank board available for the construction of a new process
Feedback and discussion	**10:00**	Give the time to present the process they just draw, confront this process whit the information in the interviews
Guidelines Part 2	**05:00**	Explain the objective of the second part of the workshop
Establish the basis for the ideal process	**20:00**	Participants should establish what would be the objectives to be achieved in an ideal process, taking into account your current process.
Feedback and discussion	**10:00**	Discussion time and feedback to research team

Tool application evaluation questionnaire

1. Nom de votre entreprise *

2. Quel est votre nom ? *

3. Quelle est votre poste dans l'entreprise ? *

Veuillez évaluer les activités réalisées en fonction des critères proposés.

Activités : Les entretiens individuels — L'atelier de formalisation — L'atelier de recommandations

4. Contenu des activités *

Une seule réponse possible par ligne.

	Pas du tout d'accord	Pas d'accord	Neutre	D'accord	Tout à fait d'accord
Les objectifs des activités étaient clairs.	⬭	⬭	⬭	⬭	⬭
Le contenu des activités était structuré et bien préparé.	⬭	⬭	⬭	⬭	⬭
La charge de travail était adaptée au objectifs.	⬭	⬭	⬭	⬭	⬭
Les activités ont été organisées de manière à ce que les participants soient pleinement impliqués.	⬭	⬭	⬭	⬭	⬭

5. Compétences et réactivité des animateurs *

Une seule réponse possible par ligne.

	Pas du tout d'accord	Pas d'accord	Neutre	D'accord	Tout à fait d'accord
Le animateur était pédagogique	⬭	⬭	⬭	⬭	⬭
Le animateur a su motiver les participants.	⬭	⬭	⬭	⬭	⬭
Le animateur a utilisé efficacement le temps dont il disposait.	⬭	⬭	⬭	⬭	⬭
Le animateur était à l'écoute des participants et disponible.	⬭	⬭	⬭	⬭	⬭

6. Comment amélioreriez-vous ces activités ? *

7. Quels éléments des activités ont été les plus utiles ou intéressants, selon vous ? *

Évaluation de l'outil en général

8. Contribution *

Une seule réponse possible par ligne.

	Pas du tout d'accord	Pas d'accord	Neutre	D'accord	Tout à fait d'accord
L'outil vous a permis de clarifier le processus de conception de produits	◯	◯	◯	◯	◯
Cette outil vous a permis d'identifier les possibilités d'amélioration de votre processus de conception de produits.	◯	◯	◯	◯	◯
Cette outil vous a permis d'avoir une vision globale du processus de conception des produits	◯	◯	◯	◯	◯
L'outil vous a permis d'évaluer le flux des ressources sur votre processus de conception de produit.	◯	◯	◯	◯	◯

9. Contribution general *

Une seule réponse possible par ligne.

	Pas du tout d'accord	Pas d'accord	Neutre	D'accord	Tout à fait d'accord
L'outil mis en œuvre est utile pour comprendre votre processus de conception de produits	⬭	⬭	⬭	⬭	⬭
Vous appliqueriez les recommandations de l'outil	⬭	⬭	⬭	⬭	⬭
La mise en œuvre des recommandations données par l'outil est pertinente pour votre équipe de conception	⬭	⬭	⬭	⬭	⬭
L'outil influencera la façon dont les produits sont conçus dans votre entreprise	⬭	⬭	⬭	⬭	⬭
En général, l'apport au processus de conception de votre produit est pertinent	⬭	⬭	⬭	⬭	⬭

10. Quels éléments de l'implémentation ont été les plus utiles ou intéressants, selon vous ? *

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11. Si vous avez d'autres commentaires, n'hésitez pas à les laisser ici

Merci beaucoup pour votre participation.

Pour plus d'informations, contactez Jose Rivera jose-luis.rivera-gil@univ-lorraine.fr

Appendix D. Summary in French

Les problèmes de conception peuvent être aussi simples que de trouver un moyen clair de communiquer un message ou aussi complexes que de mettre un satellite en orbite. Le processus de conception est à la fois une activité humaine individuelle et collective. Du côté individuel, il s'agit d'une activité quotidienne, qui doit répondre à des problèmes élémentaires ou très complexes. En tant que tâche collective, les groupes pluridisciplinaires confrontent leurs idées, leurs connaissances et leurs expériences (Boly et al., 2016). La conception d'un produit selon la théorie C-K décrit un processus dans lequel un designer pense un nouvel objet par l'interaction entre l'espace conceptuel et l'espace des connaissances. Dans ce processus, le designer explore et imagine de nouveaux concepts, puis il utilise ces connaissances pour créer des objets et de nouveaux concepts (Hatchuel & Weil, 2003).

Pour les organisations, la conception de nouveaux produits est fondamentale pour maintenir ou améliorer leurs avantages concurrentiels sur le marché (Morel & Boly, 2006) . La conception et le lancement de produits dans les organisations impliquent les activités de création, de développement et de commercialisation d'un produit qui est accepté par les clients et qui satisfait leurs besoins. Les entreprises chimiques sont confrontées à des situations différentes et à des défis particuliers selon le type de produit qu'elles conçoivent, compte tenu de la satisfaction et des contraintes du marché et du client cible qu'elles veulent atteindre (Gani & Ng, 2015).

Conception de produits chimiques : le contexte actuel

Lorsque les entreprises chimiques conçoivent un nouveau produit, elles doivent répondre de manière satisfaisante et harmonieuse aux exigences de la conception en considérant au moins trois dimensions : technique, organisationnelle et durabilité (Heintz, Belaud, & Gerbaud, 2014 ; Uhlemann et al., 2019). D'un point de vue technique, une action synergique des ingrédients et du procédé de fabrication confère les propriétés au produit. Ainsi, les combinaisons de ces variables peuvent générer un immense espace de solutions avec de multiples solutions acceptables (Filipovic et al., 2017 ; Martín & Martínez, 2013). D'un point de vue organisationnel, ce vaste espace de solutions doit être limité afin de répondre, non seulement aux attentes des utilisateurs, mais aussi aux exigences et aux désirs des autres parties prenantes, notamment celles de l'organisation où le produit est créé (Šimberová & Kita, 2020). À cet égard, le processus de conception du produit doit être aligné sur la stratégie et le plan d'organisation de l'entreprise. De plus, les produits doivent être conçus en suivant les principes de durabilité à partir de différentes dimensions : sociale, économique, environnementale, politique et technologique (Narvaez, 2014). La performance des organisations en matière de durabilité sera liée aux décisions prises lors des étapes de conception et de développement du produit. Ainsi, le contexte organisationnel dans lequel se déroule l'activité de conception du produit peut contraindre ou influencer les décisions prises par les équipes de conception.

La formulation : un processus particulier

Le processus de conception des produits chimiques de consommation d'un comprend au moins, d'un point de vue classique, les étapes suivantes : (1) la fixation de l'objectif technique, organisationnel et de durabilité, (2) la recherche des demandes des clients et leur traduction en spécifications technologiques, (3) la conceptualisation du produit, (4) la sélection des matières premières et des fournisseurs, (5) et la conception du processus de production (Cooper, 2019). Il s'agit d'un processus multi-objectifs et multi-acteurs qui pose un défi important aux entreprises, car elles doivent gérer les informations et les connaissances liées à toutes les variables de conception tout au long du cycle de conception et de développement du produit (Wang et al., 2021).

En outre, il est communément admis que la conception de produits chimiques nécessite une approche multidisciplinaire et multi-échelle (Cisternas, 2006 ; Costa et al., 2006 ; Kind, 1999) pour prendre en compte les propriétés physiques, la conception du processus et les interactions utilisateur-produit. Ainsi, la conception de produits implique la combinaison de plusieurs domaines de connaissances, notamment la thermodynamique, le marketing, les besoins des consommateurs, l'organisation commerciale, la durabilité, la territorialité et la chaîne d'approvisionnement (Fung et al., 2016 ; L. Zhang et al., 2020).

Sur la base des aspects susmentionnés, une caractéristique clé à aborder dans cette recherche doctorale est le contexte organisationnel. Le contexte organisationnel de la conception de produits implique l'interaction de multiples acteurs ayant des compétences et des responsabilités différentes (Goodwin, 2009). Ces acteurs peuvent être internes à l'organisation, comme le chef de projet, l'équipe de conception, le technicien de laboratoire, le responsable de la qualité, le responsable des achats, entre autres. Ils peuvent également être externes, comme les utilisateurs, les clients, les fournisseurs, les entités réglementaires ou les consultants externes. Le rôle des acteurs et leurs interrelations sont spécifiques à chaque entreprise et sont dynamiques au cours du développement du processus de conception. En ce sens, le processus de conception est une activité détaillée qui se déroule dans un contexte organisationnel complexe et changeant. Différentes approches peuvent être utilisées en fonction de la culture de l'entreprise pour répondre à un problème de conception similaire. En outre, le processus de conception n'est pas linéaire. Il nécessite des validations intermédiaires et de multiples cycles d'itération jusqu'à ce que le produit puisse être lancé sur le marché. Enfin, le succès d'un produit ne dépend pas seulement de la sélection correcte des ingrédients et du processus de fabrication. Tout en répondant aux exigences techniques, il doit également satisfaire aux attentes et aux exigences des parties prenantes, notamment de l'utilisateur final et d'autres acteurs tels que les organismes de réglementation, ainsi qu'à des spécifications moins bien définies, comme le fait d'être en phase avec les tendances du marché et des consommateurs.

Le manque d'inclusion du contexte organisationnel dans le processus de conception, est une opportunité de recherche pour la proposition d'un outil de conception qui considère cet aspect. Leur analyse peut permettre de comprendre quels sont les moments clés dans un projet de conception de produit, ainsi que de reconnaître les acteurs et les décisions prises à différents niveaux, de la stratégie d'entreprise à la formulation du produit.

Champ de recherche et problèmes associés

Afin de réduire le champ d'application de ce travail de recherche et en même temps de développer les lignes de recherche des laboratoires et des groupes de recherche impliqués dans ce travail, cette étude se concentre sur l'industrie cosmétique. Les produits de cette industrie sont destinés au consommateur final et la plupart des produits sont un bon exemple de produits chimiques formulés. Les industries cosmétiques opèrent dans un contexte de marchés en évolution rapide et de consommateurs de plus en plus informés et exigeants (Suaza Montalvo, 2020). Par conséquent, les entreprises qui conçoivent ces types de produits chimiques doivent réagir plus rapidement et plus précisément en lançant de nouveaux produits sur le marché pour survivre dans cet environnement très concurrentiel.

De plus, les aspects impliqués dans les projets de conception de produits, tels que la créativité, l'innovation, le travail en équipe multidisciplinaire, la prise de décision, la sélection des ingrédients, la conception du processus, la mise à l'échelle, le lancement et la vente, sont réalisés dans un contexte organisationnel. Par conséquent, les méthodologies de conception de produits chimiques doivent être alignées sur le marché dans lequel elles sont appliquées. D'après notre analyse de l'état de l'art (chapitre 2), la conception de produits chimiques est un sujet d'actualité qui a attiré l'attention des chercheurs en génie chimique. Cependant, une grande partie de la production scientifique dans ce domaine ne tient pas compte de la nécessité de considérer le contexte réel de la conception de produits chimiques : la conception de produits est effectuée dans des organisations et le résultat de la conception est limité par les ressources et les capacités des organisations où elle a lieu.

Compte tenu de ce qui précède, ce travail aborde la question de recherche suivante

Comment concevoir des produits chimiques formulés en tenant compte du contexte de l'entreprise dans le processus de conception ?

L'énoncé de l'hypothèse répondant à cette question de recherche est le suivant :

Une méthodologie de conception de produits chimiques formulés, basée sur l'analyse du système créé au sein des entreprises lors d'un projet de conception, permettra à l'équipe de conception d'avoir une perspective globale de l'ensemble du processus de conception. Cela permettra à l'équipe de conception de prendre des décisions plus éclairées aux premiers stades de la conception et de suivre une trajectoire de conception moins itérative afin de créer des produits à haute valeur ajoutée pour le client, l'entreprise et les acteurs impliqués.

Cette thèse cherche à comprendre les conditions organisationnelles qui définissent le contexte du processus de décision dans la conception de produits chimiques. Elle propose un cadre organisationnel pour appliquer les méthodologies de conception de produits chimiques existantes. L'objectif général de cette recherche est :

Proposer une méthodologie pour la conception de produits chimiques formulés dans un contexte d'entreprise.

Les objectifs spécifiques du projet sont :

- Objectif 1 : Concevoir une méthode de modélisation du système du processus de conception de produits dans les entreprises cosmétiques.
- Objectif 2 : Intégrer et analyser les besoins des parties prenantes dans le modèle de système proposé.
- Objectif 3 : Intégrer une méthodologie pour la conception de produits cosmétiques dans le modèle de système défini.
- Objectif 4 : Valider la méthodologie en modélisant un système de conception dans une entreprise (étude de cas) du secteur cosmétique.

La méthodologie générale de recherche mise en œuvre commence par la phase 1 : le cadre théorique qui démontre que les chercheurs sont de plus en plus intéressés à proposer des méthodologies pour concevoir avec plus de succès de nouveaux produits chimiques, mais ils ne considèrent presque jamais le contexte organisationnel dans toute son étendue (Rivera Gil et al., 2022). Sur la base de l’analyse bibliométrique, les objectifs présentés dans ce chapitre ont été établis. La phase 2 de la méthodologie de recherche utilise une analyse de système pour comprendre le contexte du problème de conception, les acteurs, les processus et leurs relations dans un environnement organisationnel lors de la conception de produits chimiques. Cela se fait par l'analyse de plusieurs entretiens avec des experts en formulation de produits. La phase 3 a établi une stratégie pour intégrer les recommandations pour l'amélioration du processus de conception afin de mieux répondre aux besoins des entreprises chimiques et à leur culture organisationnelle. Sur la base des résultats des phases 2 et 3, du système de conception et des recommandations répondant aux besoins de l'organisation, la phase 4 présente un nouvel outil de conception de produits chimiques qui intègre des considérations organisationnelles pour soutenir les décisions de conception. Le document contient également l'application de cette méthodologie à une étude de cas, qui permet de tester et d'obtenir des retours sur la proposition.

Contributions

Ce document fournit plusieurs contributions liées à différents domaines scientifiques dans la problématique de la conception de produits chimiques :

Déclencheurs pour la conception de produits chimiques : Une base théorique complète a été établie pour justifier ce travail. Une analyse bibliométrique des dernières publications dans le domaine de la conception de produits chimiques a été réalisée. Ces publications ont été analysées selon trois axes principaux : le type de produit, le contexte organisationnel et les phases des méthodologies de conception de produits présentées par les auteurs. Grâce à cette analyse, les bases pour le développement de cette recherche ont été établies : premièrement, il a été constaté que les produits formulés sont un objet d'intérêt pour la plupart des auteurs, parce que leur conception implique des défis scientifiques importants, et en raison de leur haute valeur ajoutée. Ensuite, les méthodologies de conception de produits manquent d'une approche intégrée qui prend en compte toutes les étapes de la conception du produit ; en particulier, l'analyse des besoins est mal comprise. Enfin, il a été constaté que le contexte dans lequel se déroule le processus de conception, c'est-à-dire le contexte de l'organisation, ses limites et ses possibilités, n'est pas pris en compte dans une large mesure lors de la proposition de méthodologies de conception.

Conception de produits chimiques dans un contexte organisationnel: Une méthodologie d'analyse du système de conception de produits a été proposée avec deux objectifs : 1) décrire le système qui est créé lorsque les organisations conçoivent des produits chimiques et 2) comprendre les besoins des organisations pour mettre en œuvre des stratégies de conception et de développement de produits. La méthodologie d'analyse a été appliquée à onze études de cas avec des experts en conception d'entreprises de différents secteurs industriels, tous ayant une expérience dans la conception de produits formulés et la plupart dans les secteurs cosmétiques. L'analyse a permis d'identifier les acteurs, les étapes de conception, les ressources et les interconnexions des éléments dans les processus de conception analysés. En outre, plusieurs particularités des systèmes de conception de produits ont été mises en évidence : Le processus de conception est spécifique à l'organisation. L'environnement organisationnel fournit des contraintes et des facilitateurs qui articulent l'équipe de conception. En outre, il s'agit d'un système qui s'étend au-delà des limites de l'organisation, en tenant compte des principales parties prenantes externes, telles que les fournisseurs et les agents de réglementation, entre autres. Notamment, les besoins des utilisateurs sont le point central de la conception du produit. Il existe un manque de clarté parmi les acteurs impliqués dans la tâche de conception, une situation qui peut générer des complications pour l'équipe de conception.

Vers une base de connaissances pour soutenir la conception de produits en tenant compte du contexte organisationnel : Ici, une base de connaissances a été créée et développée dans laquelle les connaissances partagées par les experts en conception et développement de produits chimiques sont présentées de manière organisée et exploitable. Pour cette contribution, trois étapes ont été suivies : la collecte d'informations, la création d'un cadre d'analyse, et l'extraction et la caractérisation des recommandations. La base de connaissances qui en résulte est le fondement de la construction d'un outil d'analyse du processus de conception dans les organisations. Elle contient des recommandations qui peuvent être utilisées par les organisations pour améliorer leur processus de conception. De plus, la méthodologie utilisée pour la construction de la base de connaissances est une approche qui peut être utilisée par les organisations pour stocker et organiser leurs connaissances implicites acquises par l'expérience.

Construction d'un outil pour soutenir la gestion du processus de conception de produits chimiques : L'outil proposé ici est l'intégration des contributions précédentes. L'outil vise à soutenir la conception de produits chimiques dans les organisations. Comprenant que la conception est un processus hautement dépendant du contexte, l'outil est basé sur une méthode participative qui permet aux membres de l'équipe de conception de collaborer activement à la génération et à l'évaluation de recommandations pour l'amélioration du processus de conception. L'outil se compose de trois modules : le premier, pour comprendre l'état actuel du processus de conception de l'organisation en utilisant l'approche d'analyse de système décrite ci-dessus ; le deuxième, pour extraire des recommandations pour l'amélioration du processus de conception à partir de la base de connaissances ; et le troisième, pour évaluer la pertinence des recommandations en considérant les concepts de valeur d'intérêt pour l'organisation.

Application de l'outil à un cas réel : A l'aide d'une étude de cas, l'outil proposé dans cette recherche a été appliqué avec les objectifs suivants : 1) tester le fonctionnement de l'outil, en établissant des protocoles concrets pour les entretiens et les ateliers, et 2) tester la pertinence des résultats proposés par rapport à un cas réel et une équipe de conception réelle. L'application a permis de vérifier le fonctionnement de l'outil. L'outil a permis à l'équipe de conception de connaître et de formaliser ses activités quotidiennes dans un processus formel de conception de produit. En outre, l'approche participative utilisée pour l'outil a démontré son acceptabilité, son adaptabilité et sa pertinence. En outre, les recommandations génèrent plusieurs perspectives pour améliorer leurs propres processus de conception de produits en alignement avec les concepts de valeur stratégique pour l'entreprise.

Les contributions ci-dessus répondent aux objectifs de cette recherche, qui visait à intégrer le système qui est créé dans l'organisation lors de la conception de produits chimiques, en créant et en testant un outil qui permet de mettre à jour les méthodologies de conception de produits des entreprises.

Perspectives

Compte tenu de ce qui précède, l'occasion est donnée de présenter quelques perspectives supplémentaires pour la recherche et pour l'outil proposé dans ce document.

Développement approfondi de l'outil. Dans le cadre de cette recherche, une étude de cas a été réalisée auprès d'une entreprise en France qui produit des ingrédients formulés en cosmétique. Les résultats de l'approche qualitative testée sont prometteurs et démontrent sa pertinence. Cependant, il semble nécessaire, afin de juger de la pertinence de l'outil d'un point de vue général, de tester cet outil auprès d'un plus grand nombre d'entreprises issues de différents secteurs de la chaîne de production cosmétique et présentant des caractéristiques variables dans les équipes de conception. En effet, une validation quantitative permettrait de donner de la solidité à l'outil. Cependant, une telle étude devra prendre en compte la réalité dynamique des organisations et de leurs processus.

Renforcer la caractérisation du profil de l'organisation. L'étude peut être complétée en considérant l'effet de la dimension humaine dans le processus de conception. Dans cette étude, cette dimension a été indirectement considérée en caractérisant les acteurs de la conception sous forme d'activités et de phénomènes observables dans la cartographie du système. La dimension humaine n'a pas été pleinement intégrée dans notre étude, mais elle ouvre une perspective de recherche intéressante, par exemple, dans l'étude du profil des leaders au sein des membres de l'équipe de conception. En outre, une approche de modélisation de la maturité peut être utile pour évaluer le profil de l'organisation, y compris différentes dimensions comme la dimension humaine et technologique, entre autres. L'évaluation de la maturité peut être développée sur une séquence d'étapes contenant des éléments qui décrivent les caractéristiques du profil de l'organisation à un niveau de développement donné.

Maturité de la base de données. La proposition de recommandations basées sur la base de connaissances est prometteuse, même si l'on considère qu'au moment de l'application de l'outil, elle était encore jeune et avait une participation relativement faible d'experts. Une alimentation constante de la base de connaissances ainsi qu'un traitement supplémentaire des données pourraient générer des recommandations plus adaptées. De plus, l'intégration d'experts dans d'autres domaines de connaissances est nécessaire pour étendre la base de connaissances actuelle à d'autres domaines de connaissances dans la conception et le développement de produits tels que le marketing, le développement de logiciels, l'innovation, la psychologie du consommateur, entre autres

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