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Manuscript

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Highlights:

- OntoCosmetic is an ontology for the design of emulsion-based cosmetic products.
- It contains specific concepts and their interrelations such as: cosmetic ingredients, heuristics, expert knowledge, and product properties.
- The article presents in detail the development and the elements that are part of the ontology.
- Finally, the ontology is used as a framework for decision-making in two examples of cosmetic product design.

Abstract:

The design of formulated products, such as cosmetic emulsions, requires handling heterogeneous information such as ingredients data, property models, heuristics, and theoretical knowledge, among others. Because of this, the formulation process is not straightforward, but iterative, highly intuitive, and very experimental. Our proposal to facilitate the design process is an ontology called OntoCosmetic for emulsion-based cosmetic products. An ontology is a conceptual knowledge representation of a domain. It can be interpreted by both designers and machines, allowing extensive exploration of the solution space and a logical understanding of the results of that exploration. This article presents in detail the construction of OntoCosmetic, whose structure is based on a domain ontology for Process System Engineering called OntoCAPE. Two examples show its use: the substitution of an ingredient in a formulation, and the exploration and delimitation of the solution space in a new formulation design problem.

Keywords: Ontology, chemical product design, knowledge engineering, cosmetic products, process systems engineering.

1. Introduction

Formulated chemical products, such as cosmetics, are complex systems whose properties are defined by a synergistic action of ingredients, composition, and the production process. Their design is a challenge, as it requires the management of heterogeneous information from multiple sources and the application of multidisciplinary knowledge (Zhang et al., 2020). Available information for product design is huge and diverse in nature: there are multiple ingredient databases, property models, heuristics, knowledge from colloidal science, regulations, recommendations, and guidelines, among other factors. In addition, the design must be fast and able to respond to the multiple demands of the market, which requires efficient, multifunctional, innovative, and environmentally friendly products, among other considerations. Due to their complexity, formulated products are usually designed based on expert knowledge and exhaustive experimentation, which makes it an iterative and time-consuming process (Kontogeorgis et al., 2022).

In view of the above, academia has worked extensively on the development of tools to streamline the design process of formulated products. Some renowned examples include: a methodology for formulated products based on the reverse design approach, which generates thousands of product alternatives and then filters them against a target product (Conte et al., 2011); the virtual process-product design laboratory (VPPD-Lab), which is a computer-aided tool containing property models, databases, and knowledge bases to support the design of formulated products (Kontogeorgis et al., 2022); an integrated framework for the design of formulated products containing tools and design steps for all type of formulations (solid, liquid, gas) (Zhang et al., 2017); and the computational tool ProCAPD, which combines ten sub-models (molecular structure, property, process, costing, pricing, economic analysis, quality, sustainability, environmental impact, and performance) with a database for formulated product design (Kalakul et al., 2018)(Liu et al., 2019). Most of these approaches define design problems as mathematical optimization problems of the mixed-integer nonlinear programming type (MINLP).

Despite the multiple efforts, the existing tools are not widely applied to real industrial problems (Zhang et al., 2020), and the chemical industry continues to develop products based on the experimental approach. This happens because most of the existing tools have rigid architectures based on available models and information, but not on their practical application for decision-making in real product design problems (Abbott, 2019). Most of them are generic and not easily adaptable to specific design contexts. For example, in the case of cosmetics, there is a difference between what mathematical models can predict, mainly physicochemical properties, and what formulators would like to predict, mainly stability and sensory properties (Moussour et al., 2017)(Wortel and Wiechers, 2000). Additionally, the application of existing tools requires a complete definition of the problem and full information, which is not always the case at early design stages when the problem is ill defined and information is scarce.

While recent methodologies have incorporated surrogate models and heuristics for the prediction of more properties of interest (Arrieta-Escobar et al., 2019)(Zhang et al., 2021), they are still far from representing the form in which designers think, create, and make design decisions. Beyond an automated design optimization tool to which the designer must adapt, future design support tools should be guided by the natural progression of the design process and not the other way around (Chandrasegaran et al., 2013). It is thus necessary to create tools that enable a comprehensive understanding of the solution space for its exploration and representation, which can be understood by computers to enable rapid inferences to support design decisions, make sense of the information allowing a conscious decision-making, enable communication between multiple designers understanding that design is usually multidisciplinary and collective, and can be updated to learn from each design experience.

Given the above, it is possible to say that such a functional knowledge representation for the design of a formulated product is still needed. Moreover, there is no tool with similar features for the specific case of cosmetic product design. In view of the above, this article proposes an ontology for the design of emulsified cosmetic products to explore the application of this tool in the knowledge representation of chemical product design systems.

An ontology is a knowledge management tool which seems to correspond to some of the characteristics described above to support modern design processes. As partially described in (Shen and Chen, 2012), an ontology has the following characteristics: it is semantical, conceptual, and holistic because it describes a domain by indicating the concepts and relations between the concepts that make it up as a whole (Hailemariam and Venkatasubramanian, 2010)(Sugumaran, 2016). It is machine and human readable, allowing for logical understanding by humans, as well as the drawing of inferences and the application of algorithms with the aid of computers (Marquardt et al., 2010). It is as precise as required because it is normally defined within a specific domain of knowledge and with a clear purpose (Gabriel et al., 2019).

Numerous ontologies have emerged in complex and concept-rich areas of knowledge, such as medicine, biology, and chemistry. Concrete examples are the Unified Medical Language System (UMLS®), a medical ontology to support the modeling of medical knowledge in clinical practices (Bodenreider, 2004); the Chemical Entities of Biological Interest (CHEBI), an ontology of chemical compounds in living organism (de Matos et al., 2010); and Purdue Ontology for Pharmaceutical Engineering (POPE), an ontology for pharmaceutical drug development (Hailemariam and Venkatasubramanian, 2010). In the area of chemical engineering, OntoCape stands out, which is a large ontology for the design of chemical processes (Marquardt et al., 2010). Despite the above examples, to the best of our knowledge there are no ontologies to support the design of formulated products of the cosmetic type.

In view of the above, this work proposes OntoCosmetic, an ontology to systematically represent knowledge for the formulation of cosmetic products of the homogenous mixture or emulsion type. It purpose is to support data storage and analysis, information modeling and decision-making for the design of cosmetic formulations. Its structure was inspired in OntoCape and the content is based on previous publications containing design heuristic and emulsion principles applicable to the design of cosmetics (Arrieta-Escobar et al., 2020) (Serna et al., 2021).

In this document, Section 2 presents a short introduction to ontologies and the methodology used for the development of OntoCosmetic. Section 3 explains in detail OntoCosmetics, its elements and interrelations. Section 4 presents two application cases of this ontology. Section 5 analyzes the results of the ontology. Finally, Section 6 highlights some conclusions and perspectives of the ontology.

2. Concepts and methods for the development of the ontology

2.1. Ontologies: main concepts

An ontology is a conceptual model of a knowledge domain (Gruber, 1993) . In its most basic expression, it contains at least the following three elements:

- Classes which are concepts or sets containing individuals (e.g., the class ‘Ingredient’ in a cosmetic formulation).
- Properties which are of two types: object properties relating individuals of two classes with each other (e.g., the relation ‘hasIngredient’, connecting individuals of ‘Formulation’ with ‘Ingredient’), and data properties relating an individual to a numerical or textual value) (e.g., an ‘Ingredient’ has the property ‘Melting point’, which is a real number with °C or K as units).

- Instances which are the individuals of the classes (e.g., 'Coconut oil' (INCI: Cocos Nucifera (Coconut) Oil)', which belongs to the class 'Ingredient').

Figure 1 shows an example of a basic ontology having the elements previously mentioned. These elements are the building blocks of the ontology. They allow the representation of a system as large or as simple as required by adding more or fewer blocks.

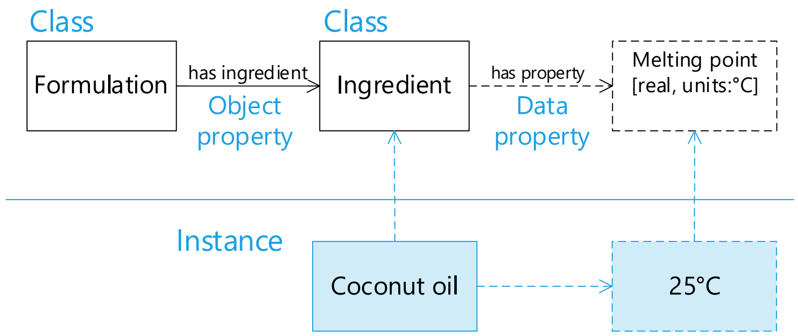

Figure 1. Example of an ontology containing the basic elements.

Once an ontology is formalized, it is possible to interact with it in multiple forms, for example by making a query to search for stored information as with any other data-base. More interesting is to use a reasoner to perform logical inferences. The reasoner can look for implicit information and logical inconsistencies based on the definitions explicitly made in the ontology. Additionally, it is also possible to apply logical rules to classify or reclassify instances within the ontological model.

Ontologies are part of semantic web technologies as shown in Figure 2. The purpose of these technologies is to make internet data, which is mostly semantic, machine readable. Thus, the utilization of these technologies has the potential to enable access to an immense source of information, specific and contextual, that is not normally considered in traditional approaches.

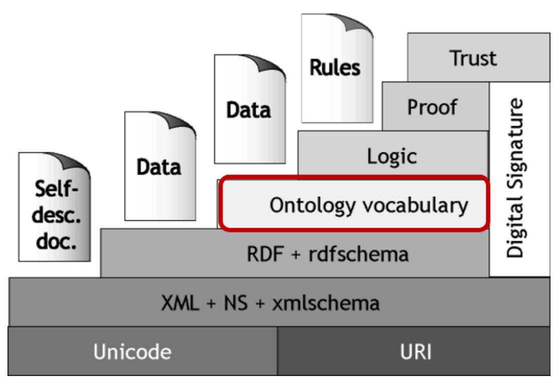

Figure 2. Semantic web stack (Berners-Lee, 2000)

According to the level of generality, ontologies can be classified into representation ontologies, generic (or common) ontologies, top-level (or upper-level) ontologies, domain ontologies, task ontologies, method ontologies, and application ontologies (Guarino, 1998)(Gomez-Perez et al., 2004). As an information system (IS) aims to support human activities, symbols used in this IS to describe the specific world of the organization and its process constitute a symbolic ontology (Guarino, 1998). The writing and use of this ontology lead to an ontology-driven information system (Guarino, 1998). The ontology can be used to affect the IS components – application programs, databases, user interfaces – in such a way as to accomplish a concrete (business) purpose (Guarino, 1998).

2.2. Methodology

There are various methodologies in scientific literature to structure the process of designing an ontology. The first guidelines for ontology design were proposed by Gruber (1993), Gruninger and Fox (1995), who introduced the stages of definition of a scope, identification of concepts, semi-formal and formal representation of the knowledge domain and implementation of the ontology. The historical reference in ontology design methodologies is the work proposed by Uschold and Gruninger, who explicitly proposed a methodology for the development of ontologies (1996). Subsequently, Fernandez-Lopez et al. proposed METHONTOLOGY, a detailed guide to build domain ontologies (1997). Extended and varied methodologies with different steps, details, applications, focused on different aspects such as collaborative development, or high reusability, have emerged since then. Remarkable examples are the “Ontology Development 101: A Guide to Creating Your First Ontology” (Noy and McGuinness, 2001), which is a clear guide for the construction of ontologies using Protégé, and the work of Bachimont et al. (2002),which shows how to structure domain taxonomies within ontologies.

In (Gabriel, 2016; Gabriel et al., 2019) the previously mentioned methodologies among others were reviewed and summarized in the iterative methodology for ontology development shown in Figure 3. It has four main steps: 1) definition of the scope, goal, and competencies ; 2) conceptualization; 3) development; 4) validation/evaluation. The present article followed those steps which are briefly explained below:

1. Definition of scope, goal, and competencies: The scope refers to the domain as well as the level of detail described by the ontology. The goal is the purpose for which the ontology is built. It is associated with questions about competencies, which explain what is expected from the ontology. They are targets expressed in the form of questions that the ontology should be able to answer.
2. Conceptualization: All relevant concepts are listed in a table of concepts until they are sufficient to describe completely the scope of the ontology. Relations between concepts are reviewed and systematically listed. There are two types of relations (as already shown in Figure 1): relations between concepts and data properties. The information used to make the model comes from the literature or from experts, depending on the domain to be structured. Likewise, the ontology can be compared to, or based on, existing ontologies. Existing ontologies are available in the literature or in ontology repositories such as LinkedOpenVocabulary (https://lov.linkeddata.es), among others. In addition to the reuse of domain specific ontologies, it might also be interesting to use upper level ontologies to increase interoperability of the ontology with other ontologies and tools (Elmhadhbi et al., 2018).
3. Development: This step refers to converting the ontology into a language that can be read by the computer. In this case, the ontology was modeled using Protégé (Musen, 2015) and the versioning (record of the different versions of the development process) was done using GitHub (https://github.com/ERPI-UL). The documentation was generated with Widoco (Garijo, 2017). The reasoner Pellet was selected because it is compatible with the SWRL language (Parsia et al., 2005; Sirin et al., 2007). The SWRL language was used to work with design rules (heuristics).
4. Validation/evaluation: The evaluation is done in three levels: first, the syntaxis is checked and the consistency of the ontology is examined with the reasoner; secondly, the ontology is compared against the target competency -questions; thirdly, the ontology is evaluated with a case study. For the first evaluation level, the reasoner engine is used to detect and correct error messages. For the second evaluation level, competencies are converted to SPARQL queries and then they are used in

the ontology to check if it provides the expected results. The ontology is iteratively improved until it meets all conditions and can answer all competency -questions. For the third evaluation level, a case study is developed implementing the ontology for the purpose for which it was built. In the case of OntoCosmetic, it is built to support design decisions.

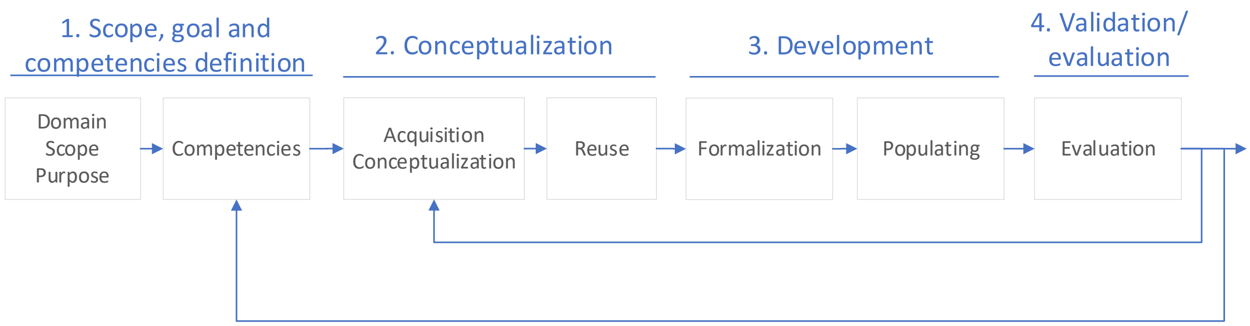

Figure 3. Methodology for the generation of the ontology. Schema from (Gabriel et al., 2019).

The ontology was developed in collaboration between experts in cosmetic product formulation and ontology engineers as suggested in (Kotis et al., 2020). Several versions of the ontology were developed and validated until the current version was reached. The following sections show in detail the development of the ontology.

3. Results

The main result of this work is the creation of the ontology for the formulation of cosmetic products.

3.1. Ontology scope and competencies

The scope of OntoCosmetic is the formulation of emulsion-based cosmetic products. The long-term purpose of this ontology is to create a decision support system for cosmetic product formulators. This version of the ontology addresses two types of cosmetic design decisions: the substitution of an ingredient and the exploration of the solution space for a new cosmetic product. For this, the ontology should describe ingredients, formulations (including the composition of ingredients), design heuristics, and their interrelations. Table 1 presents a list of target questions about competencies.

Table 1. Main competencies that OntoCosmetic must answer.

ID	Competencies
C1	Given a certain property, which substance possesses it?
C2	Given a formulation, what is its composition (dosage)?
C3	What are the formulation rules (heuristics) that are related to a given ingredient type?
C4	What is the impact of heuristics on a formulated product?
C5	Given a formulation, what are the heuristics it fulfills?

3.2. Conceptualization result

3.2.1. Conceptualization bases

The conceptualization of OntoCosmetic was based on cosmetic product formulation literature, exchanges with expert and existing ontologies from the chemical engineering domain. The structure of the ontology was based on the works of (Arrieta-Escobar et al., 2020) (Serna et al., 2021). Some concepts were also extracted from the following ingredients supplier guides: (Mentel et al., 2014), (Croda, 2013), (BASF, 2012), (Croda, 1998), (ICI Americas Inc, 1980). The conceptualization was done iteratively with exchanges between experts in product formulation and ontology engineers in a collaborative approach as recommended in (Kotis et al., 2020). Additionally, according to the "reuse" principle, the ontology OntoCape (Marquardt et al., 2010) was used to enrich the conceptualization process of OntoCosmetic. OntoCape is a large-scale ontology for the domain of Computer Aided Process Engineering (CAPE) with multiple abstraction levels (Marquardt et al., 2010). Figure 4 presents a fragment of the conceptual level of OntoCape representing technical systems.

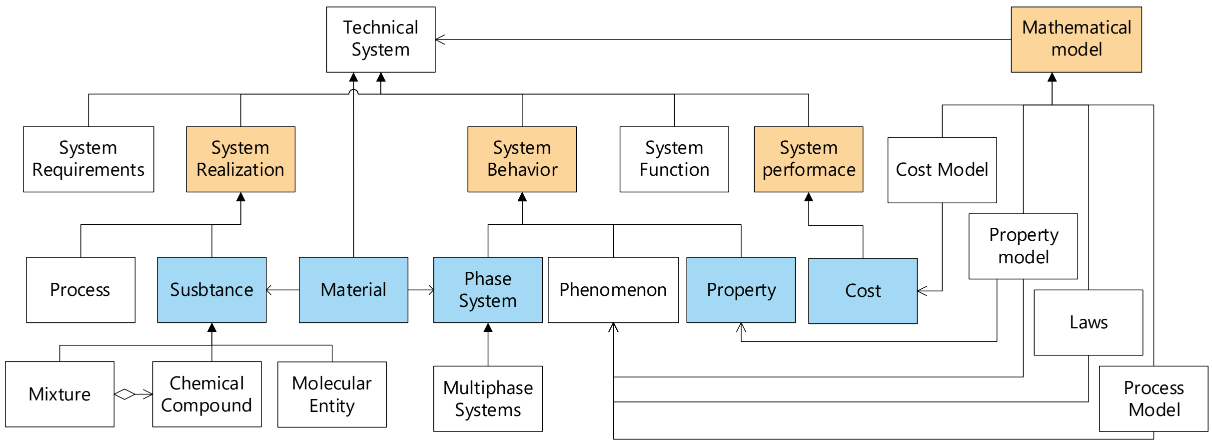

Figure 4. Partial representation of the Technical System concepts from OntoCape. Based on information from (Marquardt et al., 2010).

OntoCape defines technical systems as products or processes developed in an engineering design process. They are represented through five viewpoints: requirements, function, realization, behavior, and performance. OntoCosmetic adapted the following concepts from OntoCape to represent cosmetic formulations:

- "System realization", which corresponds to the decisions that designers can make and implement to meet product requirements. It has the modules of process and substances, which can be translated to OntoCosmetic as the fabrication process and substances comprising ingredients and formulations, respectively.
- "System behavior", which corresponds to the real behavior of the system. It can be characterized through system properties. It can also be related to a phenomenon, or a phase system (which can be a single phase in homogeneous systems or multiphase in heterogeneous systems). These concepts can be adapted to OntoCosmetic to represent substance properties and substance micro-structure.
- "System performance", which evaluates the design system in relation to design requirements. The evaluation is normally done through indicators. Examples are cost indicators, performance indicators, and sustainability indicators.
- "Mathematical models", which describe equations that model the behavior of the systems. Based on these models, it is possible to relate the system realization to the systems behavior and performance. In OntoCosmetic mathematical models predict the effects of design decisions in the formulation properties. In addition to mathematical equations, OntoCosmetic considers design heuristics.

Based on the previous analysis, the conceptualization of OntoCosmetic uses four main concepts: 1) substance, its subclasses and its properties (sections 3.2.2 and 3.2.3), 2) property and property state (Section

3.2.4), dosage (related to the composition of the formulation) (Section 3.2.5) and heuristic (Section 3.2.6). Figure 5 represents the relationships between these concepts.

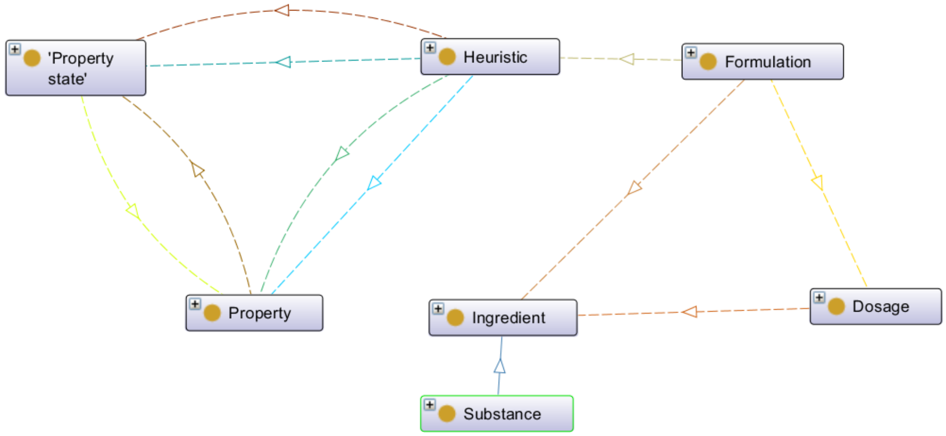

Figure 5. Overview of the main elements of OntoCosmetic.

3.2.2. Substances and their subclasses

Any entity within the ontology, including substances, processes, and products, is described as a system. The term substance refers to any chemical entity (pure or mixture). Process is a set of chemical or physical transformations that converts raw materials into products. Product is a designed substance that is ready to be released on the market. This version of the ontology deals specifically with the substance class and its subclasses. For this purpose, the concept is divided into four main subclasses, as illustrated in Figure 6: Pure substance is a substance that cannot be decomposed. Mixture represents all the substances composed of more than one pure substance. Ingredient is the constituent unit of the formulation. It can be a mixture or a pure substance. Formulation is a combination of ingredients with their composition. Additionally, the ingredient class has the subclasses surfactants, emollients, and thickeners, among others. Table 2 lists all the concepts of this hierarchy with their meanings.

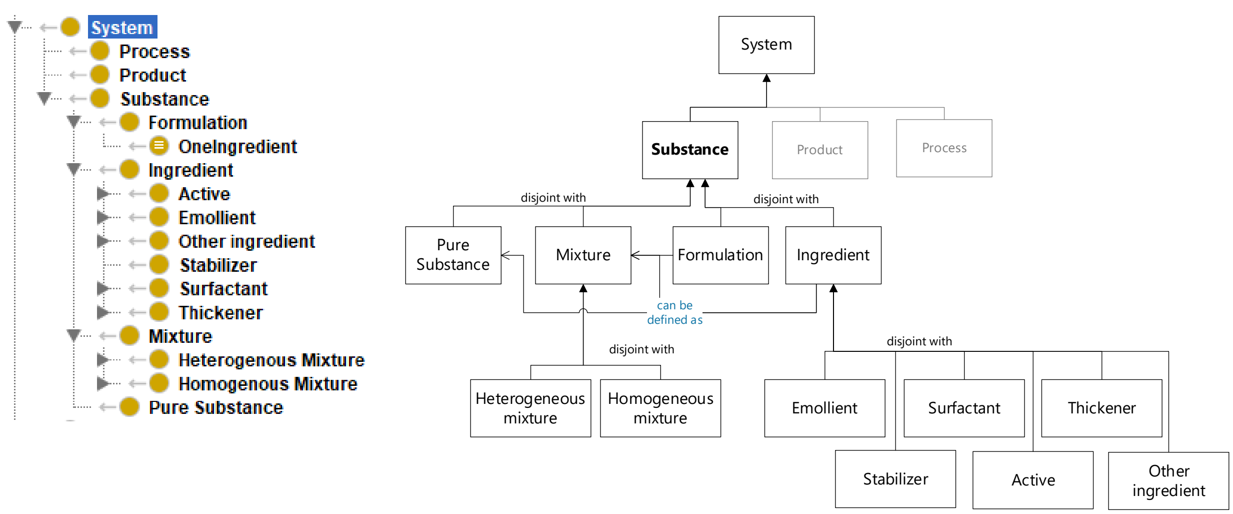

Figure 6. Extract from OntoCosmetic and diagram of the hierarchy of the class 'Substance' and its subclasses.

Table 2. List of concepts related to substance and its subclass.

Concept	Description
Substance	Any chemical entity (pure or mixture).
Mixture	An entity made up of one or more substances. It can be homogeneous or heterogeneous.
Pure substance	A single substance that cannot be separated into other substances by any physical means.
Formulation	A designed mixture of ingredients. It can be homogeneous (solutions) or heterogeneous (colloidal system). It contains a list of ingredients with a composition (dosage)
Ingredient	Constituent unit of the formulation.
Emollient	Ingredient of oily nature used in cosmetics to make skin and hair softener. Additionally, it can be used for the following purposes: as a solvent for liposoluble actives, as an occlusive ingredient to prevent water loss from the skin. Emollients can be classified according to their chemical nature: ester, fatty alcohol, fatty acid, hydrocarbon, silicon, or triglyceride.
Surfactant	Ingredient that lowers the interfacial tension between two immiscible phases. It is used in emulsions for three purposes: to decrease the energy required for emulsification, to adsorb rapidly at the interface of recently formed droplets, and to generate a barrier, either electrostatic, steric, or both, for long-term emulsion stability. Additionally, it can be used as an active ingredient in cleaning products such as soaps, shampoos, and in surface conditioners. They can be classified according to their electrical nature, as nonionic, ionic-anionic, or ionic-cationic.
Thickener	This is a substance that can significantly modify the rheology of a fluid. Thickeners are added to the formulation for three main purposes: to increase viscosity, to promote a particular rheological behavior (pseudo-plastic, thixotropic, among others), and to enhance emulsion stability.
Active	Ingredient that performs a specific function on the skin. Examples are humectants, antioxidants, anti-aging ingredients, sun filters, and pigments, among others.
Stabilizer	Ingredient used to avoid or reduce droplet coalescence.
Other ingredient	Ingredient with another function, different from those already performed by previous classes described. Examples are preservatives, chelating agents, colorants, fragrances, and pH regulators, among others.

3.2.1. Properties

Figure 7 lists an extract of the object and data properties used to conceptualize the formulation process. Table 3 shows object properties and Table 4 shows data properties. Some properties are common to all the ingredients such as ‘has origin’ (which indicates if an ingredient is natural, is produced from natural raw materials, or is synthetic) or ‘chemical nature’ (which classifies a substance considering inorganic and organic chemical categories, such as ester, ether, etc.). Other properties are specific to a category of ingredient such as ‘HLB’ for surfactants and ‘emollience’ for emollients.

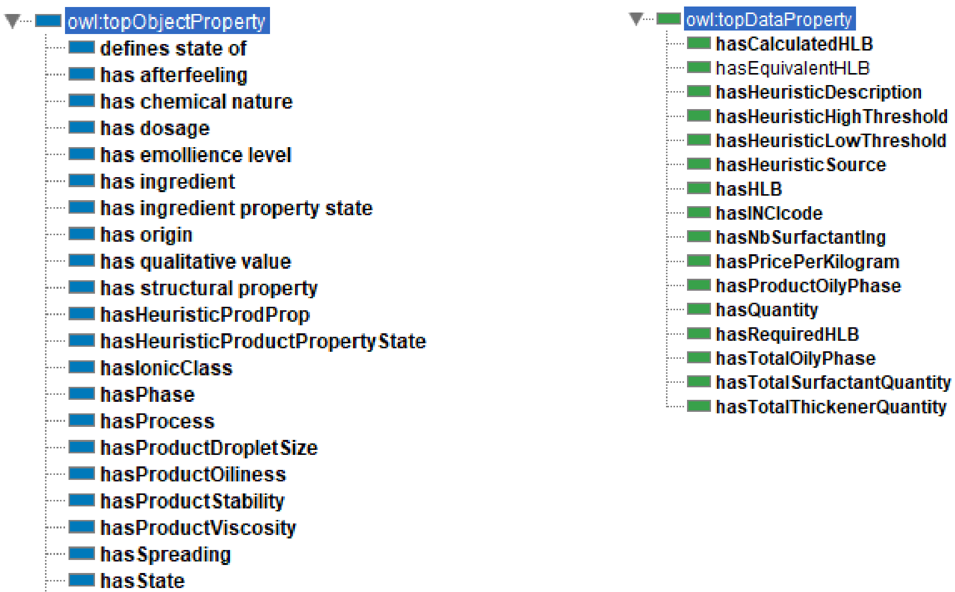

Figure 7. Extract of the OntoCosmetic - object and data properties (object properties in blue, data properties in green).

Table 3. Extract of the list of object properties of OntoCosmetic.

Property name	**Description**	**Domains**	**Ranges**
has chemical nature	Refers to the chemical nature of an ingredient	Ingredient	Chemical nature
has phase	Defines in which phase the ingredient is soluble	Ingredient	Phase state
has origin	Provides the origin of an ingredient	Ingredient	Origin type
has emollience level	Gives the level of emollience of an ingredient of the emollient type	Emollient	Emollience level
has after feeling	Gives one or several after feeling properties to an ingredient of type emollient	Emollient	After-feeling state
has spreading	Defines the spreading property of an emollient	Emollient	Spreading state
has ionic class	Defines the ionic nature of an ingredient	Surfactant	Ionic state
has texture	Provides the texture that can be expected from a given surfactant	Surfactant	Texture state
has ionic class	Defines the ionic nature of an ingredient	Surfactant	Ionic state

Table 4. Excerpt from the list of data properties of substances and their subclasses.

Property name	**Description**	**Domains**	**Ranges**
has HLB	Quantifies the HLB of a surfactant	Surfactant	Float
has INCI code	Defines the INCI code of a cosmetic ingredient	Ingredient	String
has price per kilogram	Price per kilogram of an ingredient	Ingredient	Float
has product oily phase	Percentage of the formulation that is part of the oily phase.	Formulation	Float
has required HLB	Quantifies the required HLB that of an emollient.	Emollient	Float

3.2.2. ‘Property’ class and ‘Property state’ to describe qualitative characteristics

Some substance properties are qualitative and enable the classification of the substances in subclasses. For example, the property ‘Spreading’ of an emollient, which is related to the ability of the emollient to spread on the skin, can take the following qualitative values: very high, high, between medium and high, medium, between medium and low, and low. Thus, emollients can be classified in the categories of very high spreading emollients, high spreading emollients, etc.

Thus, to describe qualitative properties, it was necessary to create two classes: the class ‘Property’ and the class ‘Property state’. The class ‘Property’ is a qualitative characteristic of a substance (e.g., Spreading). This class is instantiated by individuals that are the qualitative values of the property and are called ‘Property state’ (e.g., possible spreading states are very high, high, between medium and high, medium, between medium and low, and low). These two concepts, which take the form of classes in the ontology, are different from the object and data properties mentioned earlier.

The class ‘Properties’ is connected to the different classes of ‘Substance’ by the object property ‘is property of’. Figure 8 illustrates the hierarchy of the classes related to the class ‘Property’.

Table 5 summarizes the object properties associated with the class ‘Property’.

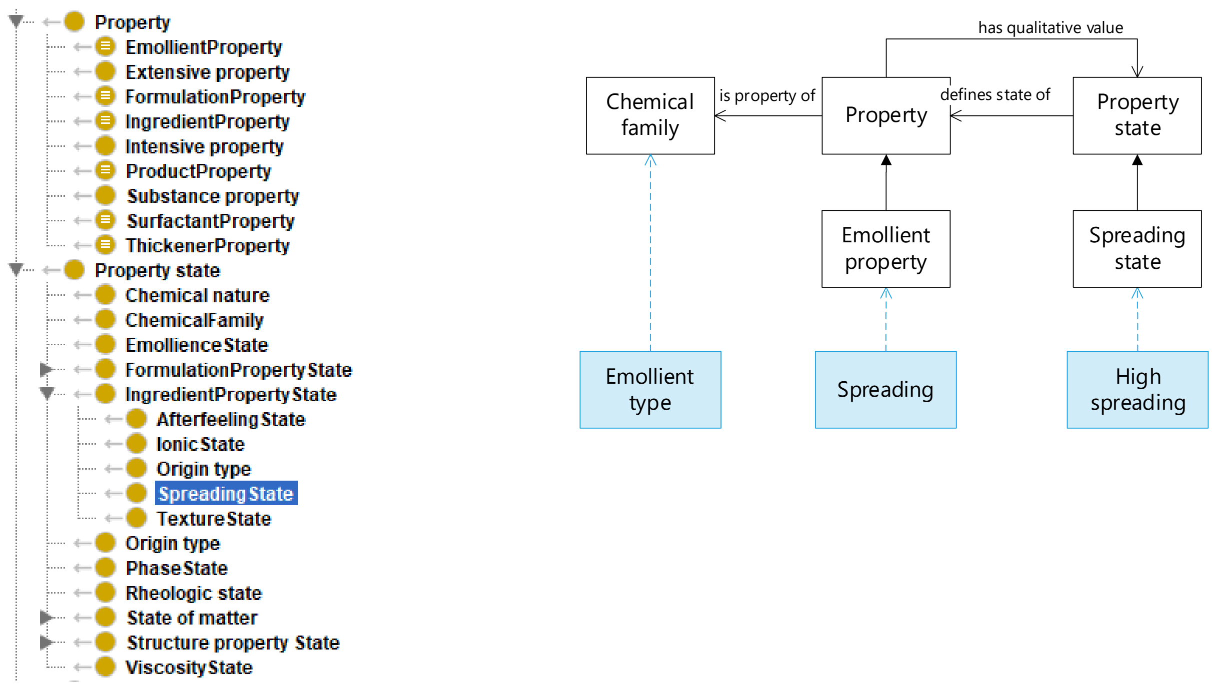

Figure 8. OntoCosmetic extract and diagram of the class ‘Property’ and the class ‘Property state’.

Table 5. List of object properties related to property.

Property name	Description	Domains	Ranges
defines state of	Relationship between the qualitative state of a property and the property	Property state	Property
has qualitative value	Inverse relation of ‘defines state of ‘. It links a property to its qualitative value	Property	Property state
is property of	Defines the type of substance (chemical family) that is concerned by the property	Property	Chemical family

3.2.3. Formulation and dosage: list of ingredients and their composition

The main scope of the ontology is to represent the formulation process, which consists of the determination of the ingredients and their composition. To represent this action, the ontology introduces the 'Dosage' class. It is the combination of an ingredient and its quantity in a formulation. It has two properties: 'is quantifying' which relates the dosage to an ingredient, and 'has quantity' which connects the dosage to the percentage by mass of that ingredient. A formulation is related to several individuals of 'Dosage' through the property 'has dosage'. Figure 9 shows a representation of this and other properties of the class 'Formulation'. Table 6 and Table 7 summarize all properties of the 'Formulation' class.

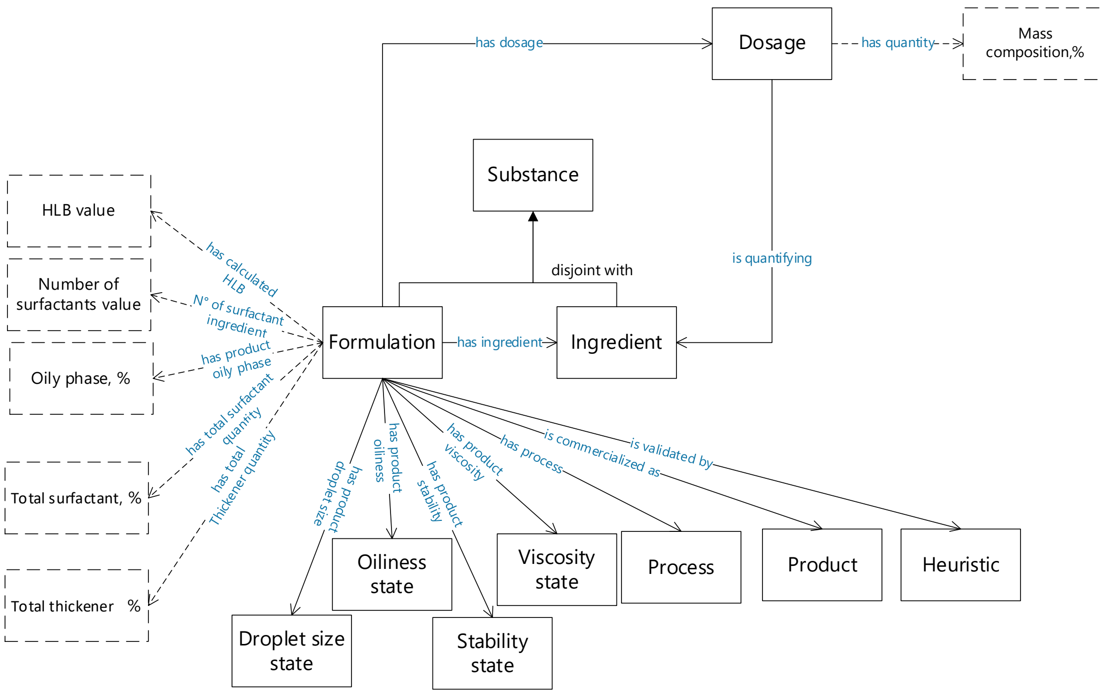

Figure 9. Diagram of the relation between formulation and dosage.

Table 6. List of object properties related to 'Formulation' and 'Dosage'.

Property name	Description	Domains	Ranges
is quantifying	Assigns an ingredient to a dosage	Dosage	Ingredient
has dosage	Assigns a group of dosages to a formulation	Formulation	Dosage
has ingredient	Defines the ingredients that are used in a formulation	Formulation	Ingredient
has product droplet size	Defines the average droplet size of a formulation. The droplet size depends on the formulation and the process.	Formulation	Droplet size state
has product oiliness	Defines the oiliness of a formulation	Formulation	Oiliness state
has product stability	Defines the stability of a formulation	Formulation	Stability state
has product viscosity	Defines the viscosity of a formulation	Formulation	Viscosity state
has process	Assigns a process (sequence of step) to a formulation	Formulation	Process
is commercialized as	Relates a formulation with a product that is or will be commercialized	Formulation	Product
is validated by	Indicates the heuristics that the formulation follows.	Formulation	Heuristic

Table 7. List of data properties related to formulation and dosage.

Property name	Description	Domains	Ranges
has quantity	The quantity of ingredients that compose the dosage. This quantity is in percentage of volume of the formulation.	Dosage	Float

has calculated HLB	The final HLB of the surfactant mixture that compose the formulation	Formulation	Float
N° of surfactant ingredient	Define the number of surfactants in a given formulation.	Formulation	Integer
has product oily phase	Percentage of the formulated product that represents oily ingredients.	Formulation	Float
has total surfactant quantity	The total quantity of surfactant that a formulation has. This quantity is in percentage of volume.	Formulation	Float
has total thickener quantity	The total quantity of thickener that a formulation has. This quantity is in percentage of volume.	Formulation	Float

3.2.4. Heuristic: validating the formulation

The class 'Heuristic' defines the design rules that product formulators use to predict the effects of design decisions. Heuristics are linked to several classes. First, a heuristic is related to the trigger of the rule, which can be the presence of an ingredient type in the formulation (emollient, surfactant, etc.), an ingredient property and/or a property value. Secondly, the heuristic is related to the impact of the application of the rule, which is expressed in a product property and a product property value. Some heuristics have a quantity threshold to trigger the rule, which means that they are only active when a certain property value is achieved. To indicate this, heuristics have two data properties: 'has heuristic high threshold' and 'has heuristic low threshold', which compare a formulation value with an inferior and superior threshold, respectively, to determine the activation of the rule.

As an example, the heuristic C33 of the data base states: "Viscosity is high (cream to gel texture) if a high proportion of thickener is used (0.5 to 1%)". It is related to the ingredient 'Thickener' and its dosage as activators. The latter is compared to the heuristic thresholds to define its activation. Additionally, the heuristics C33 is also related to the product property 'Viscosity' and the viscosity state of 'high' as effect. Figure 10 shows heuristic properties. Table 8 and Table 9 list them.

Table 8. List of object properties related to the 'Heuristic' class.

Property name	**Description**	**Domains**	**Ranges**
has ingredient property state	Defines a relation between a heuristic and a specific state of a property. It defines the property state that could trigger the heuristic.	Heuristic	Property state
has heuristic product property state	Define the state that is given to the property when the heuristic is verified.	Heuristic	Property state
has heuristic product property	Associate a heuristic with a product property. The rule has an impact on the properties of the final product formulated.	Heuristic	Property
is affected by ingredient property	Associate a heuristic with the ingredient property that is involved in the rule	Heuristic	Property
involves ingredient type	Define which ingredient type is concerned with the heuristic	Heuristic	Chemical Family
has structural property	Associate a heuristic with the structure property of the formulation final product that is involved in the rule	Heuristic	Droplet size state

Table 9. List of data properties related to the class 'Heuristic'.

Property name	**Description**	**Domains**	**Ranges**
has heuristic description	Provides a description of the heuristic.	Heuristic	Literal
has heuristic high threshold	High threshold for a heuristic.	Heuristic	Float
has heuristic low threshold	Low threshold for a heuristic.	Heuristic	Float
has heuristic source	Provides the source of the heuristic (from literature or experience)	Heuristic	Literal

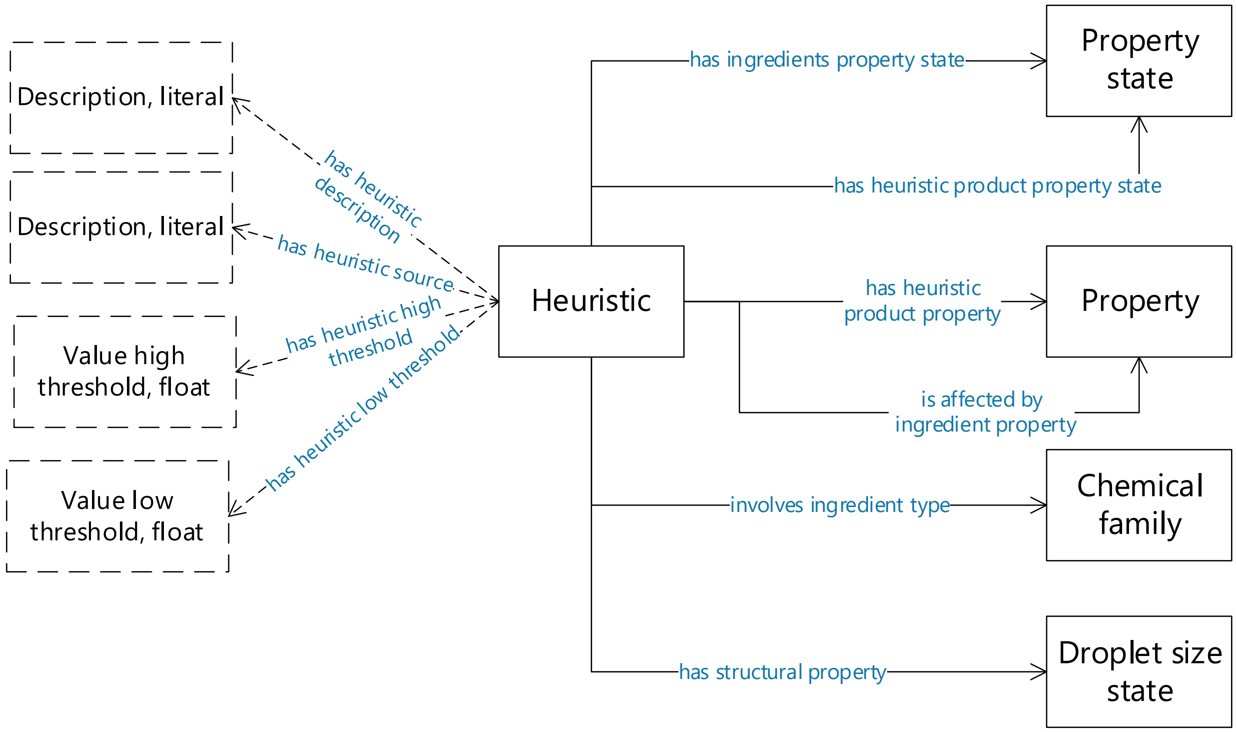

Figure 10. Diagram of the class 'Heuristic' and its properties.

The ontology contains the main concepts explaining heuristics, but the rules are formally defined outside the ontology, through axioms in the SWRL language connected to the information of the ontology.

3.3. OntoCosmetic development result

The documentation of the ontology was done with Widoco (Garijo, 2017) and is accessible online (https://purl.org/ontocosmetic). The ontology has 955 axioms, counting all the classes and the necessary instances to describe the qualitative states of properties. Figure 11. shows a graphical model of OntoCosmetic.

To enable the use of the ontology to support design decisions, it was necessary to instantiate it with ingredients data, heuristics data and formulations data to constitute a usable knowledge graph. Once fully instantiated, the ontology counts 2712 axioms. Table 10 presents metrics of the ontology and the knowledge graph.

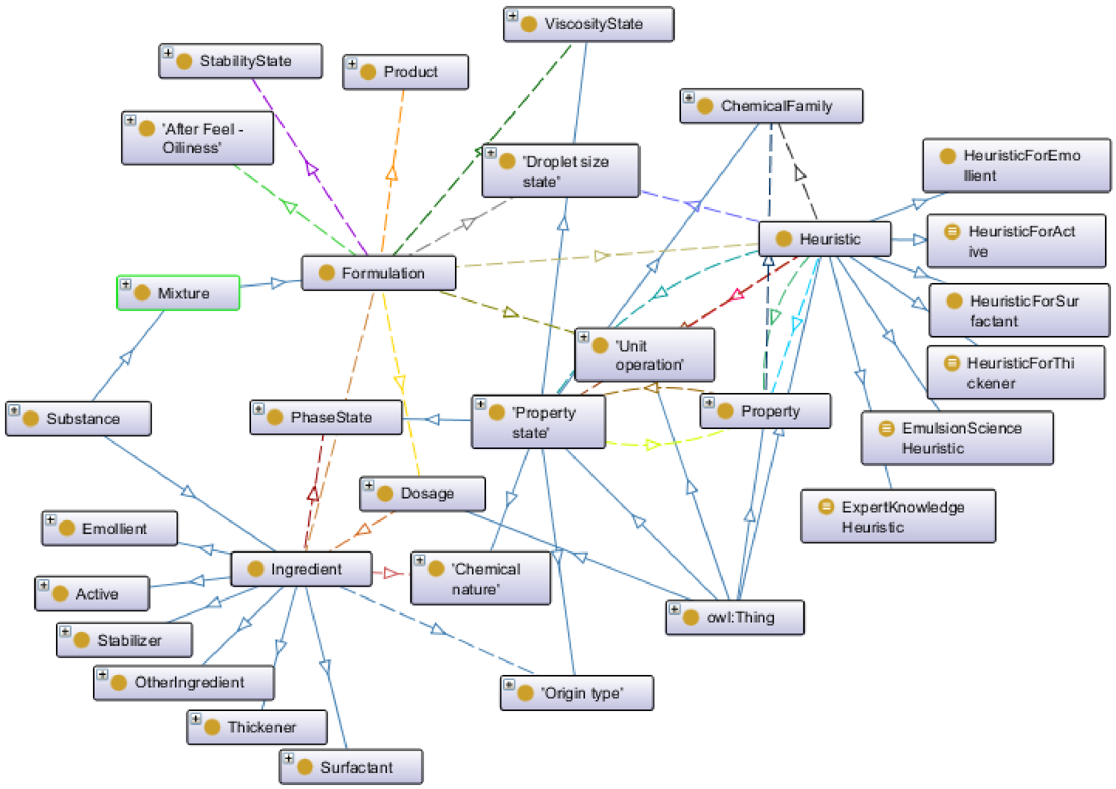

Figure 11. Overall representation of OntoCosmetic.

Table 10. OntoCosmetic - ontology and knowledge graph metrics.

Metrics	**OntoCosmetic ontology**	**OntoCosmetic knowledge graph**
Axiom	955	2712
Logical axiom count	397	1744
Class count	100	100
Object property count	32	32
Data property count	24	24
Individual count	118	340
Annotation property count	11	11

3.4. Ontology validation/evaluation

According to the methodology in Section 2.2, the first evaluation level is to run the inference engine and check for possible logic errors. This was done with each version of the ontology, which was developed in an iterative form. The second evaluation level consists of the validation of the competency-questions proposed in Table 1 by means of SPARQL requests. Table 11 illustrates the translation of the competencies into SPARQL request examples.

Table 11. SPARQL requests associated with competencies.

ID	**Competencies**	**Example of SPARQL requests**
C1	Given a certain property, which substance possesses it?	Example: Find the substance with the property HLB:

		PREFIX cosme: <https://purl.org/ontocosmetic#> SELECT ?substance WHERE { ?substance :hasHLB ?value}
C2	Given a formulation, what is its composition (dosage)?	Example: Find the ingredients and composition of a certain formulation: PREFIX cosme: <https://purl.org/ontocosmetic#> SELECT ?ingredient ?quantity WHERE { cosme:original cosme:hasDosage ?dos. ?dos cosme:isQuantifying ?ingredient; cosme:hasQuantity ?quantity.}
C3	What are the formulation rules (heuristics) that are related to a given ingredient type?	Example: Find the list of heuristics with a relation to the ingredient type 'Surfactant': PREFIX cosme: <https://purl.org/ontocosmetic#> SELECT ?heuristic WHERE { ?heuristic cosme:hasHeuristicIngType cosme:surfactant_type.}
C4	What is the impact of heuristics on a formulated product?	Example: Find the list of heuristics with a relation to the ingredient type 'Surfactant': PREFIX cosme: <https://purl.org/ontocosmetic#> SELECT ?heuristic ?productPropertyImpacted ?impact WHERE { ?heuristic cosme:hasHeuristicProdProp ?productPropertyImpacted; cosme:hasHeuristicProductPropertyState ?impact.} ORDER BY ?productPropertyImpacted
C5	Given a formulation, what are the heuristics it fulfills?	Example: Find the list of heuristics that meets a certain formulation: PREFIX cosme: <https://purl.org/ontocosmetic#> SELECT ?formulation ?heuristic WHERE { ?heuristic cosme:hasValidated ?formulation.} ORDER BY ?formulation

4. Application Case

Another way to validate the ontology is to test its purpose. To do so, a decision support system prototype in interaction with the OntoCosmetic knowledge graph was created. This prototype of ontology-driven information system is a web application made using Python and the OwlReady2 library (Lamy, 2017). The source code is available on GitHub (https://osf.io/nwzhg/?view_only=3805837fed264669a4c24e7109faa7a9). Two scenarios tested the decision support system: 1) the substitution of one ingredient and 2) the exploration of the solution space based on heuristics to identify design opportunities. The following subsections will present the two scenarios of the application case.

4.1. Substitute an ingredient

This scenario simulates the situation where a formulator would like to substitute an ingredient to satisfy new design requirements without significantly changing the properties of the product. A common example is to change an ingredient or a group of ingredients of synthetic origin for ingredients derived from natural resources.

Table 12 presents an example formulation, called original formulation, which has two ingredients that are partially synthetic: an emollient, ethyl hexyl palmitate, and a surfactant, PEG-20 sorbitan monostearate. This formulation was entered in the web application with the interface shown in Figure 12.

Table 12. Ingredients and proportion of the formulation used for the application case – original formulation

N	Class	Ingredient	[%]	Phase	Origin
1	Emollient	Ethylhexyl Palmitate	4	Oily phase	Natural and synthetic raw materials
2	Emollient	Olive oil	3	Oily phase	Natural
3	Emollient	Caprylic/Capric Triglyceride	9	Oily phase	Natural raw materials
4	Surfactant	PEG-20 sorbitan monostearate	1.9	Oily phase	Natural and synthetic raw materials
5	Surfactant	Sorbitan Monostearate	2.1	Oily phase	Natural raw materials
6	Preservative	Cosgard	0.7	Oily phase	Organic (Ecocert)
7	Antioxidant	Tocopherol	0.5	Oily phase	Natural raw materials
8	Humectant	Glycerin	3	Water phase	Natural
9	Thickener	Xanthan gum	0.1	Water phase	Natural
10		Water	75.7	Water phase	-

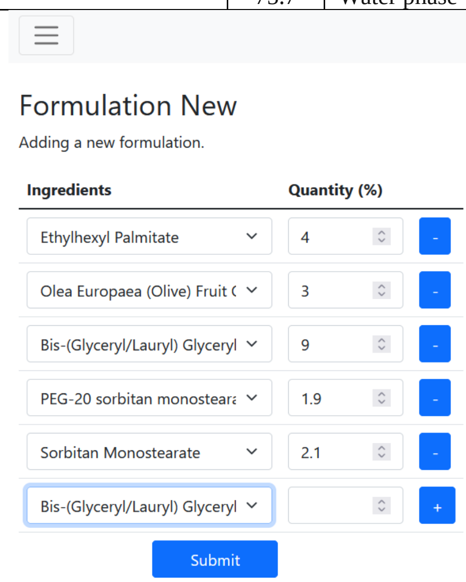

Figure 12. Screenshot of the formulation entry form in the web application.

For the replacement of the problematic ingredients, the following decision steps were performed using the ontology as information support:

1. Calculation of the properties of the original formulation: Quantitative data of the original formulation were calculated based on its composition. Examples of these are total surfactant quantity, total thickener quantity, HLB of the surfactant system, required HLB of the oily phase, etc. Then, the inference engine used these data to identify the heuristics matched by the original formulation. And subsequently, those heuristics were used to infer the properties of the original formulation, which are shown in Figure 14. It should be noted that the property viscosity has two values: It is low according to the heuristic C31 which considers the amount of thickener, and high according to heuristic C8, which considers the effect of a surfactant (sorbitan monosterate). To know which of the two heuristics has a greater effect on the viscosity, the formulation should be experimentally tested.

Product Properties

Stability	Stable
Oiliness	-
Viscosity	High viscosity, Low viscosity,
Absorption rate	Medium absorption rate
Sensorial profile	-
Total Surfactant Qte	4.0
Total Thickener Qte	0.1
Nb Surfactant	2
Total Oily Phase	21.20
Formulation price (for 1 Kg)	4.53
Formulation HLB	9.54
Formulation Required HLB	9.50
Emollient/surfacant balance (HLB/RHLB)	1.00

Satisfied Heuristics

ID	Description
A1	An emulsion tends to be more stable using a suitable combination of surfactants with a HLB equivalent to the HLB required by the emollients.
A2	It is recommended to use more than one surfactant.
C22	If most of the emollients are of medium absorption, product absorption sensation is medium, If most of the emollients are of medium absorption
C31	Viscosity is low (lotion texture) if a low proportion of thickener is used (between 0 to 0.1% for xanthan gum).
C8	Viscosity increases if surfactants recommended for creamy texture are used (For example, surfactants with long chain alkyl groups or with the stearate group tend to increase viscosity)., Viscosity increases if surfactants recommended for creamy texture are used (For example

Figure 13. Screenshot of the software prototype showing properties and heuristics of the the original formulation

2. Select possible candidates to replace the ingredient(s): Ingredients with properties similar to those of the ingredients to be replaced are identified with a SPARQL query using Protégé. Normally, there are no ingredients with the same characteristics as the original, thus the formulator must prioritize which are the most important characteristics.
   For the replacement of the emollient, the formulators decided to select natural or natural derived emollients with a price similar to or lower than the original, and with the same qualitative sensorial profile. Based on these criteria, the SPARQL query was defined (Figure 14). Two emollients were kept: Caprylic/Capric Triglyceride and Coco-Caprylate/Caprate. Table 13 presents their information in relation to the original emollient.

```
SELECT ?emollient
WHERE { ?emollient rdf:type cosme:Emollient;
cosme:hasSpreading cosme:medium_spreading;
cosme:hasEmollience cosme:light_emollience;
cosme:hasOrigin cosme:natural_raw_material.}
```

Figure 14. Example of SPARQL request used to identify candidates for replacement

Table 13. Candidates for emollients to replace Ethylhexyl Palmitate

INCI	**Class**	**Polarity**	**Viscosity**	**Spreading**	**Emollience**	**Origin**	**Price ($/kg)**	**HLB r**
Caprylic/Capric Triglyceride	Triglyce ride	Medium to high	Medium	Medium	Light	Natural raw materials	16	11
Coco-Caprylate/Caprate	Ester	Medium	Medium	Medium	Light	Natural raw materials	15.9	9.3
To be replaced: Ethylhexyl Palmitate	Ester	Medium	Medium	Medium	Light	Natural and synthetic raw material	17.2	8

For the surfactant, the formulators decided to select naturally derived surfactants with high HLB (superior to 10) to favor an oil in water (O/W) emulsion and with a similar or lower price than the original molecule. Two surfactants were kept: Glyceryl Stearate Citrate, Glyceryl Stearate SE. Table 14 shows them.

Table 14. Candidates of surfactants to replace PEG-20 sorbitan monostearate.

INCI	**Price ($/kg)**	**HLB**
Glyceryl Stearate Citrate	20.1	12
Glyceryl Stearate SE	11.2	12
To be replaced: PEG-20 sorbitan monostearate	23.7	14.9

3. Create formulation candidate: Using the previously selected ingredients, four formulations were proposed by combining all surfactant-emollient pairs. Except for the Candidate 1, which will serve as a non-optimized example, the compositions of surfactants were corrected to correspond to the required HLB of the emulsion. Table 15 show all formulation candidates.

Table 15. Comparative table of the original formulation and formulation candidates

		Original	**Candidate 1***	**Candidate 2**	**Candidate 3**	**Candidate 4**
Ingredient		[%]	[%]	[%]	[%]	[%]
Emollients	Olive oil	3	3	3	3	3
	Ethylhexyl Palmitate	4				
	Caprylic/Capric Triglyceride	9	13	13	9	9
	Coco-Caprylate/Caprate				4	4
Surfactants	PEG-20 sorbitan monostearate	1.9				
	Glyceryl Stearate Citrate		1.9		2.8	
	Glyceryl Stearate SE			3.0		2.8
	Sorbitan Monostearate	2.1	2.1	1.0	1.2	1.2
Others	Cosgard	0.7	0.7	0.7	0.7	0.7
	Tocopherol	0.5	0.5	0.5	0.5	0.5
	Glycerin	3	3	3	3	3
	Xanthan gum	0.1	0.1	0.1	0.1	0.1
	Water	75.7	75.7	75.7	75.7	75.7

*In this case the require HLB of the oily phase does not correspond to the HLB of the surfactant system to illustrate the use of the prototype

4. Validate formulation candidates in relation to heuristics: All four candidates were inserted in the decision support system. The heuristics allowed the determination of the properties of the different candidates. Figure 15 shows that all the formulations have similar properties. However, Figure 16 shows that Candidate 1 does not validate the heuristic A1 related to the formulation stability. The ontology does not point out that this candidate may not be stable because its logical functioning does not allow deductions from the non-compliance of heuristics (this is discussed later in section 5).
Finally, Figure 17 summarizes all numerical indicators of the formulations. According to Figure 17, all the specifications are the same except for the price and the HLB-RHLB ratio. In conclusion, a great alternative to the original formulation is Candidate 2. It validates the same heuristics as the original formulation, has the same expected properties, and has a price slightly lower than the original.

Formulation properties

Formulation	Stability	Oiliness	Viscosity	Absorption rate	Sensorial profile	Actions
candidate1	Stable	-	High viscosity, Low viscosity,	Medium absorption rate	-	
candidate2	Stable	-	High viscosity, Low viscosity,	Medium absorption rate	-	
candidate3	Stable	-	High viscosity, Low viscosity,	Medium absorption rate	-	
candidate4	Stable	-	High viscosity, Low viscosity,	Medium absorption rate	-	
original	Stable	-	High viscosity, Low viscosity,	Medium absorption rate	-	

Figure 15. Screenshot of the formulation properties from the decision support system.

Heuristics validation

Name	A1	A2	A3	B11	B12	B13	C11	C12	C2	C21	C22	C23	C31	C32	C33	C4	C5	C6	C7	C8	Actions
candidate1	-	✓	-	-	-	-	-	-	-	-	✓	-	✓	-	-	-	-	-	-	✓	
candidate2	✓	✓	-	-	-	-	-	-	-	-	✓	-	✓	-	-	-	-	-	-	✓	
candidate3	✓	✓	-	-	-	-	-	-	-	-	✓	-	✓	-	-	-	-	-	-	✓	
candidate4	✓	✓	-	-	-	-	-	-	-	-	✓	-	✓	-	-	-	-	-	-	✓	
original	✓	✓	-	-	-	-	-	-	-	-	✓	-	✓	-	-	-	-	-	-	✓	

Figure 16. Screenshot of the table of the heuristics validated by the formulation.

Fomulation specification

Name	Price ($US per Kg)	Total Surfactant Qte	Nb Surfactant	Total Thickener Qte	Total Oily Phase	HLB/RHLB balance	High emollience qte	Med emollience qte	Low emollience qte	Actions
candidate1	4.582	4.000	2	0.100	21.200	0.797	3.000	13.000	0.000	
candidate2	4.424	4.000	2	0.100	21.200	0.993	3.000	13.000	0.000	
candidate3	4.763	4.000	2	0.100	21.200	0.998	3.000	13.000	0.000	
candidate4	4.589	4.000	2	0.100	21.200	0.998	3.000	13.000	0.000	
original	4.535	4.000	2	0.100	21.200	1.005	3.000	13.000	0.000	

Figure 17. Screenshot of the specification table from the decision support system.

4.2. Solution space exploration using heuristics

The second application case scenario consists of the exploration of the solution space using heuristics. It responds to the need of the formulator to get to know different strategies to intentionally tune a property according to product specifications. The approach is complementary to the one shown in Section 4.1: it does not use the heuristics to calculate the properties of a formulation, but rather to identify the appropriate ingredients/strategies that will respond to product specifications. Using an application based on the ontology (Figure 18), the designer can select a property class and/or a property state to find the associated heuristics. The heuristics may lead to a list of ingredients that help to satisfy product specifications.

An example is to identify all possible strategies that would lead to a high-viscosity formulation using the application. As a result, the application shows the heuristics related to the class property 'viscosity' and to the property state 'high', which correspond to: 1) the use of a high proportion of thickener, 2) the use of fatty alcohols (such as cetyl alcohol, cetearyl alcohol and stearyl alcohol), and 3) the use of surfactants that enhance a creamy texture.

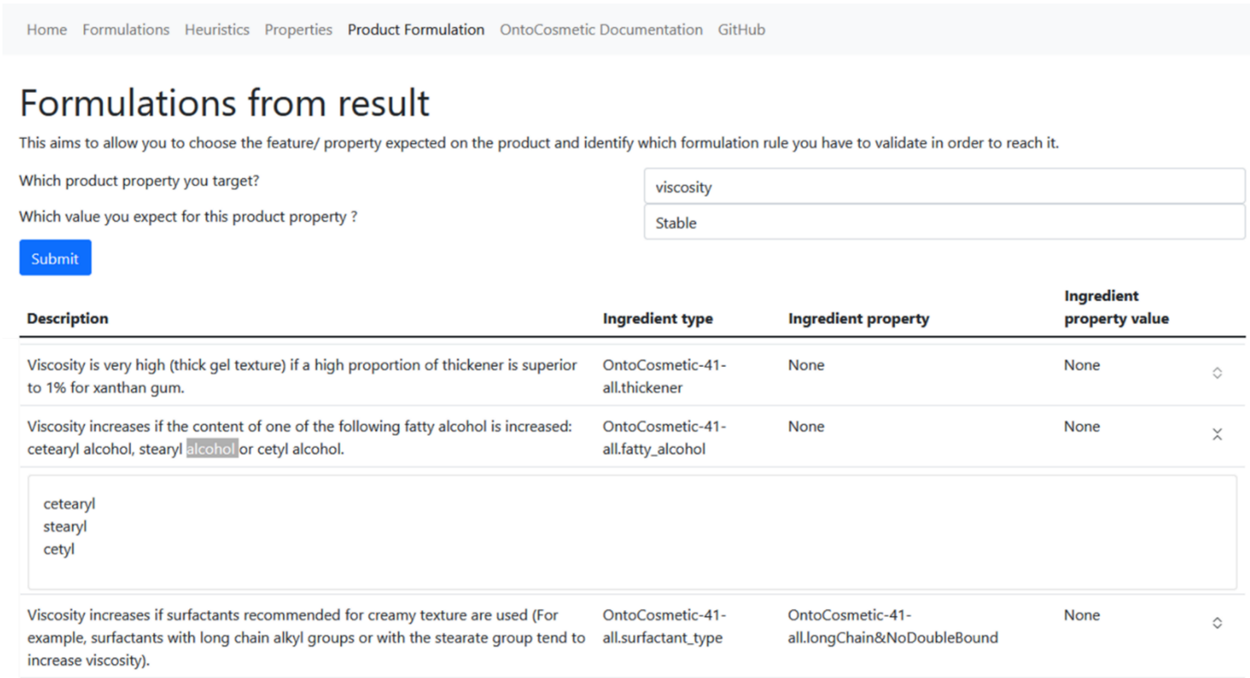

Figure 18. Screenshot of the result of the decision support system when selecting "viscosity" heuristic with high value.

5. Discussion

The above sections presented the development of OntoCosmetic as well as two application scenarios. The ontology was built based on a competency-questions methodology, which is a common approach for ontology development. However, the first results showed that this approach may have limitations: the competency-questions did not allow an assessment of whether the ontology satisfies its expected purpose, which was its use in decision support systems.

To evaluate this use, it was necessary to create a functional prototype of the intended decision support system, which in turn involved major changes to the initial version of the ontology: Firstly, it was necessary to create a knowledge graph based on OntoCosmetic using data from the literature. Secondly, an algorithm for the application of the heuristics using SWRL rules and the information in the knowledge graph was programmed. Finally, it was necessary to introduce new data properties into the ontology to store the intermediate values calculated for the application of the SWRL rules.

The authors of this article used Python 3, the dedicated library Owlready2 (Lamy, 2017), and Flask for the development of the decision support system prototype. These choices were made considering the experience of the authors in these tools to simplify the application development process. The goal was to rely as much as possible on the reasoning and inference capabilities of OWL and Pellet to validate the real potential of the ontology. Python only allowed the connection between the data introduced by the user and the ontology. Specifically, the python application loads the information from the knowledge graph, calculates essential quantitative data such as mass percentage ratios, and stores the new information in the knowledge graph to start the inference engine.

The result of this development is the current version of OntoCosmetic and a functional prototype of the design support system that uses the ontology and rules in the SWRL language for the application of design heuristics. The generation of the prototype allowed the identification of some technical limitations that should be resolved in future versions: when introducing new formulations into the knowledge graph, the python application can generate errors in the ontology that are difficult to identify. Possible alternatives to solve this issue are: 1) to verify the data before they are saved in the knowledge graph and 2) to save the formulations in separate OWL files. The first solution consists of avoiding the creation of a buggy assertion before putting it into the knowledge graph. To do so, there is language known as Shapes Constraint Language - SHACL (https://www.w3.org/TR/shacl/) which allows the creation of constraints to verify the graph (Labra Gayo et al., 2018). The second solution consists of keeping the original OntoCosmetic knowledge graph without modifications and creating a separate OWL file for each new formulation. The choice of one of the two alternatives depends on their processing time. The inference system already took between six and seven seconds to make the calculations for the five formulations of the first application case.

Beyond the technical aspects, the implementation of OntoCosmetic in a decision support system has some conceptual limitations that should also be addressed in future versions. For example, it was not possible to reach certain conclusions using the inference system of the ontology due to the open world assumption in ontology systems. According to this assumption, “what is not known to be true or false might be true. In other words, the absence of information is interpreted as unknown information, not as negative information” (Keet, 2013). As a result, the current version of the ontology can only infer that a formulation may be stable when it meets the conditions for stability, but it cannot infer that a formulation may be unstable when it does not meet the conditions. It is logical from the ontology perspective but confusing for the formulator. It is therefore necessary to use more precise heuristics to arrive at the most complete definition of the formulation properties.

Additionally, the current version did not consider heuristics or models involving manufacturing process variables. From this perspective, the ontology must be completed to handle process variables and aspects related to the micro-structure of the formulation. Furthermore, the database of ingredients is not as complete as required for accurate application of the heuristics. For example, some ingredients do not have defined data thresholds and cannot be analyzed in relation to certain heuristics. This means that, for the upcoming versions, the ingredients data properties must be extended. Finally, when more than one heuristic is related to the same product property, it is possible to obtain more than one value for that property. This was the case with viscosity in the first application case. To solve this, it is necessary to do further research to weight the effects of the different heuristics when they impact the same property.

In spite of the current limitations, the ontology together with the prototype decision support system demonstrated their potential in the two case studies discussed. Although the decision support system is still a prototype, there is no doubt that its use can have benefits for formulators. The system should be further tested with formulators to help them solve real design problems.

6. Conclusions and future work

This article presented in detail the development of the ontology OntoCosmetic, which is a conceptual model to support the design of emulsion-based cosmetic products. The ontology has four main concepts: substance, property, dosage (which refers to the composition of the formulation), and heuristics. It can describe the relation between ingredient properties and product properties through the implementation of heuristics or design rules. The novelty of this ontology is that it represents in detail the domain of cosmetic formulations and it enables the implementation of design heuristics programmed in a semantic/logical language.

This work presented several results: the ontology itself; the knowledge graph containing information about ingredients, heuristics, and example formulations; and a prototype of a decision support system that applies the knowledge graph. Additionally, the ontology has been made publicly accessible.

The decision support tool was tested through two scenarios: the replacement of ingredients in a sample formulation and the exploration of formulation strategies with the objective of achieving a target property. These scenarios enabled the authors to identify the contributions and limitations of the proposed ontology. An important contribution was the combined use of the knowledge graph with the SWRL language that facilitates the application of design heuristics. A limitation of the current version is that it does not consider the effect of process variables on product properties.

In view of the above, the forthcoming work will have three directions: Firstly, the databases will be expanded and updated following a continuous learning strategy. Secondly, the ontology will be expanded to represent aspects not considered in this version, specifically process variables. This is not a simple task because it requires adapting the concept of temporality to the current ontology, as well as a precise understanding of the effects of the process variables on the microstructure and on the properties of the formulation. Thirdly, the decision support tool will be tailored to suit the needs of the formulator. For the latter, the authors plan to perform user experience studies (UX studies) to characterize formulators' behavior and create a tool that responds to their needs and practices.

Finally, the use of ontologies has the potential to enable the application of digital technologies to support the design of formulated chemical products and to leverage current computational resources in the development of innovative new products. Additionally, the use of similar ontologies can be extended to other formulated products beyond the cosmetic sector, such as food and pharmaceuticals.

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