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Decision making software for cosmetic product design based on an ontology

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Abstract

The design of formulated chemical products such as cosmetic emulsions is normally carried out by interdisciplinary teams that need versatile and reliable tools to support them in the decision-making process. In view of this, this article presents a tool to support product designers during the conceptual design of emulsified cosmetic products. The tool is based on a previously developed ontology for cosmetic product design. It integrates concepts from emulsion science, cosmetic formulation, expert knowledge, and design heuristics in a systematic and flexible way. Additionally, it has a modern architecture based on mobile applications which makes it easy to use. The tool support three types of decisions: screening of ingredients, selection of ingredients considering multiple criteria (ingredient performance, origin, price, etc.), and evaluation of a formulation according to design heuristic. As a result, the tool allows the visualization of ingredient properties and a better selection of ingredients, as well as an early evaluation of formulations prior to experimentation.

Keywords: Product design, Cosmetic emulsions, Software application, Ontology

1. Introduction

The design of cosmetic products is a complex task that involves the management of multiple and heterogeneous information: raw material data, mathematical models, design heuristics, emulsions science principles, experimental data, among others (Zhang et al., 2020) (Kontogeorgis et al., 2022). Thereby, tools capable of handling varied information and comprehensively representing the solution space of design options are needed. They would have the potential to assist product designers in making decisions to seek original and context-specific solutions. Those tools should be flexible to be adapted to different design problems, easy to use and understand to help rather than hinder the design process, and reliable to be effective in supporting decision making.

There have been extensive contributions from the academy to produce tools for chemical product design. Some of the most notable are ProCAPD with an emphasis on the prediction of physicochemical properties for product optimization (Kalakul et al., 2018) and the virtual process-product design laboratory (VPPD-Lab) which contains a wide

database of property and molecular design models to support design decisions (Kontogeorgis et al., 2022). Previously mentioned tools are generic and not specific for cosmetic design. They are mostly applicable for the definition and resolution of optimization design problems, i.e., they can be used when the design problem is or can be well and explicitly defined. Additional examples of practical tools to support formulators in the design of cosmetics are the app-based resources from Abbott (2022), which shows how scientific principles of colloidal science can be used to explore design solutions for different formulated products, mainly paints, and the commercial software Ansys Granta MI for material design and selection (Ansys, 2022).

However, the drawbacks of the contributions are their complexity, their lack of specificity for cosmetics and their low accessibility and ease of use. In view of the above, this article presents a cross platform decision-making tool for the design of emulsion-based cosmetics at early stages. It is called Formultools. Its architecture was inspired by the OntoCosmetic ontology (Serna et al., 2022), whose scope is the formulation of emulsion-based cosmetic products.

2. Design methodology

Considering the premise that the tool must be accessible, a great importance was given to the interaction with the user/formulator. The design process was inspired by the 5-plans user-centered design approach (Garrett, 2011). It involved cosmetics experts and computer scientists in co-design. The development was done iteratively with intermediate usability tests with non-expert users. Each experience was assessed through a questionnaire using the method AttrakDiff (Lallemand et al., 2015) to follow usability improvement at each iteration. The problems encountered were progressively corrected until the current version was released.

2.1. Tool scope and functionality

The decision-making tool targets cosmetic product designers (the user). It is to be implemented at the early design stages. Three purposes were defined: the exploration of ingredients according to their properties; the selection of ingredients considering specific criteria, the evaluation of a possible formulation according to design heuristics.

3. Formultools: an application for the design of cosmetic products

3.1. Ontology as a foundation

The ontology OntoCosmetic is a knowledge representation containing all the concepts used for the development of the application. The ontology scope is the formulation of emulsion based cosmetic products. It is based on four main concepts: ingredients, formulations (list of ingredients with composition), properties, design heuristics, and their interrelations. Figure 1 presents an overview of the ontology:

- **Ingredients and formulation (dosage):** These concepts correspond to the variables that designers can select to achieve expected product properties, i.e., they are the independent variables because designers can select ingredients and their composition (dosage). Ingredients can be emollients, surfactants, thickeners, actives, other ingredients (stabilizers, preservatives, etc.).
- **Properties:** There are product properties and ingredients properties, and they characterize the behavior of the product and of the different ingredients respectively. Some properties are specific to a category of ingredient such as the HLB for surfactants. Some properties are quantitative (as the HLB) or qualitative (as the origin of ingredients, which can be natural or synthetic). As an example, Table 1 presents a list of the properties of emollients and their characteristics.

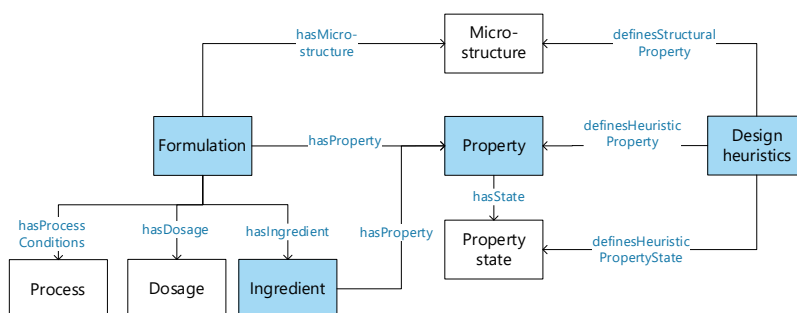


Figure 1. Overview of OntoCosmetic

Table 1. Main emollient properties in OntoCosmetic

| CAS | Meaning | Range |
|-----------------------------|--|--------|
| INCI name | Abbreviation for International Nomenclature of Cosmetic Ingredients | String |
| Chemical class | chemical nature of an emollients: ester, fatty alcohol, hydrocarbons, silicones, triglyceride, fatty acid | String |
| Polarity (qualitative) | It determines the types of inter-molecular forces of the substance. | |
| Viscosity (qualitative) | Resistance of a fluid to the deformation | |
| Spreading (qualitative) | It identifies the easy of a fluid to spread on a surface | |
| Emollience (qualitative) | It indicates if an emollient produces a light skin feel or a rich skin feel | |
| After feeling (qualitative) | It indicates if an emollient leaves an oily residue after application | |
| State | indicates if the substance is liquid or solid. | |
| Biodegradability | It is the capacity for biological degradation of organic materials by living organisms | |
| Origin | It makes refer to the source of the substance: if it is of petrochemical origin or natural origin. | |
| Price | Ingredient cost | Float |
| HLBr | It represents the HLB needed by an oil or a mixture of oils to be more likely to be incorporated in a stable O/W emulsion. | Float |
| MW | Mass of a compound divided by the number of moles | Float |

- Design heuristics: They are design rules based on expert knowledge and they relate ingredients, ingredients properties and the formulation with product properties and their values. They enable to predict the effects of design decisions in product properties. As an example, Table 2 presents a list containing some of the design heuristics.

Table 2. Example of design heuristics in OntoCosmetic

| Product property | Heuristic |
|------------------|---|
| Stability | An emulsion tends to be more stable using a suitable combination of surfactants with a HLB equivalent to the HLB required by the emollients |
| Stability | It is recommended to use more than one surfactant |
| Stability | The quantity of surfactant should be between 14 to 20% of the total oily phase |
| Viscosity | Viscosity is low (lotion texture) if a low proportion of thickener is used |
| Viscosity | Viscosity is high (cream to gel texture) if a high proportion of thickener is used |
| Viscosity | Viscosity increases if the content of one of the following fatty alcohol increases: cetearyl alcohol, stearyl alcohol or cetyl alcohol |
| Viscosity | Viscosity is decreasing if a branched-chain higher alcohol is added |

3.2. Formultools: a cross platform tool based on OntoCosmetic

Ontologies are great for formalizing knowledge but they are not intended for end users. Formultools aims to provide user-friendly interface to product designers who wants to

explore the design space at early design stages looking for product concepts to be tested. It was developed to be simple, accessible, useful, and versatile. Its data architecture is directly inspired by the OntoCosmetic ontology as the knowledge graph used is an instantiated version of OntoCosmetic with ingredients, heuristics, and properties. The structure of the application is split into two main sections as represented in **Erreur ! Source du renvoi introuvable.**. An exploration section, which is focused on ingredients searching within a collection, visualization, and ranking. And a formulation section calculating product properties based on heuristics for their verification. Its interface is inspired on mobile applications.

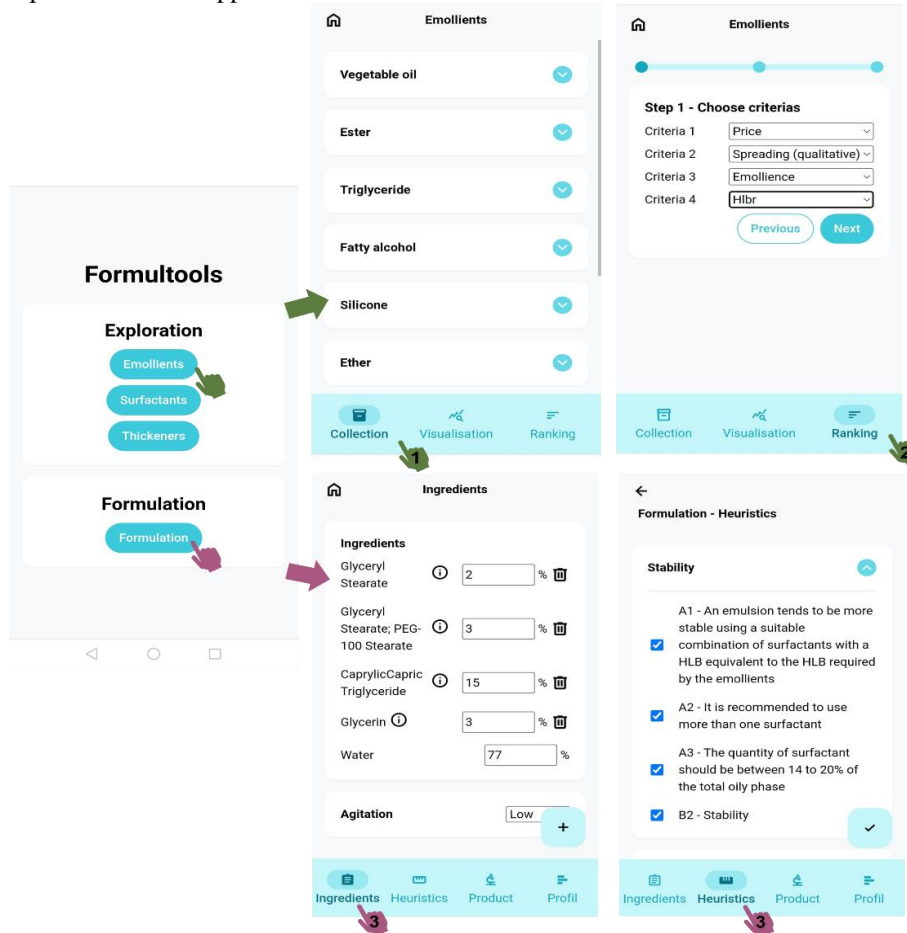


Figure 2. General interface of Formultools

The main functions of Formultools are explained below:

- **Ingredient searching and visualization:** The application has three categories of ingredients according to their functions in cosmetic products: emollients, surfactants, and thickeners, which can be accessed in the home page. Subsequently, the collection of ingredients of each category are listed and presented according to their chemical class. Ingredients can be explored in the following two ways: they can be viewed with their individual properties on the collection tap, they can be explored based on the

values of their properties and compared graphically on the visualization tap. The latter also presents the filter option, where ingredients can be screened according to their properties.

- Figure 3 presents the exploration options.

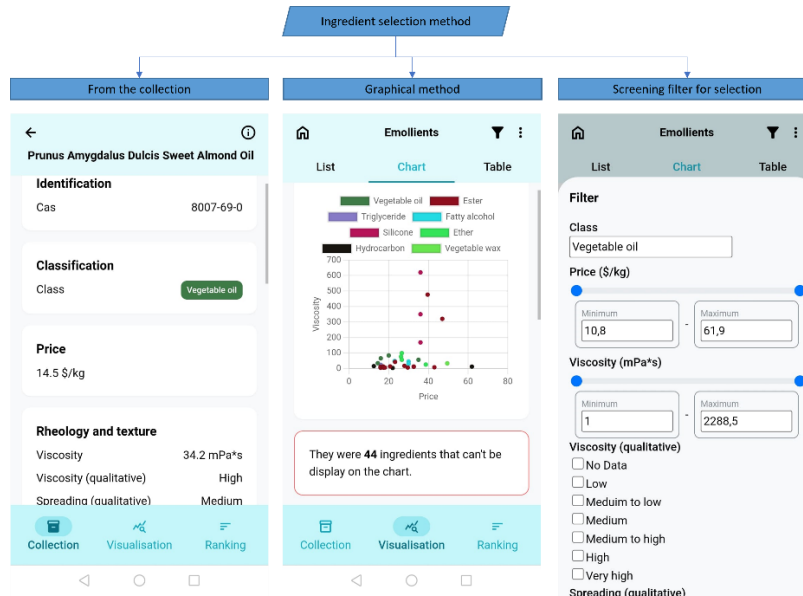


Figure 3. Exploring emollients using Formultools (collection, visualization, filter)

- **Ingredient selection:** The application enables the ranking of ingredients considering the properties that the designer wants to optimize. For this, the method Analytic Hierarchy Process (AHP) (Saaty, 1987) is used. With the aid of the tool, the formulator first defines the proprieties considered as criteria of selection in the first tap. Then, he defines which proprieties must be minimized and maximized in the second tap. Thirdly, he makes a pairwise comparison of proprieties to calculate their weights. The AHP method implies the calculation of a consistency ratio to evaluate the pairwise comparison, which can be also visualized. The last step is the visualization of the ranking. The four steps of ingredient selection are illustrated in Figure 4.

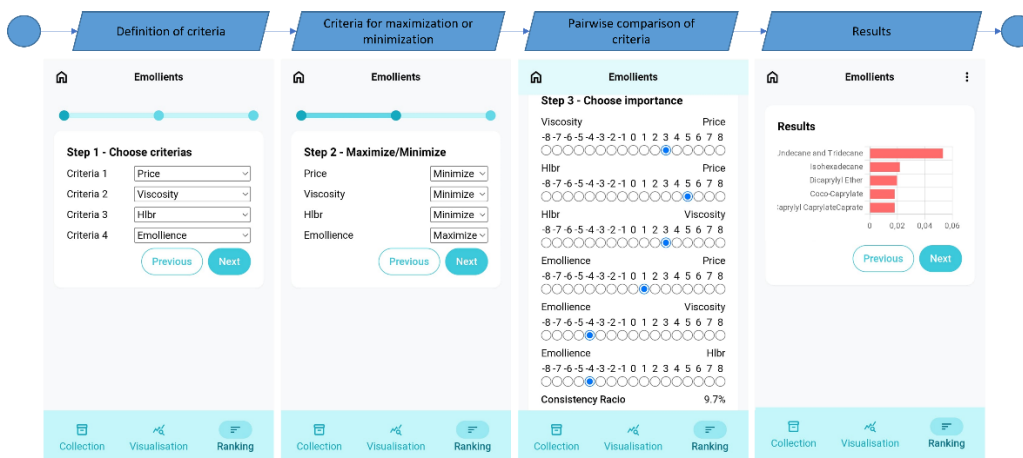


Figure 4. Ranking process of cosmetic ingredients using Formultools

- **Formulation evaluation:** FormulTools enables the evaluation of formulations suggested by designers according to design heuristic and recommendations contained in the data base. He defines a formulation (ingredients and composition), select design heuristics from the data base and based on the heuristics, the tool calculate product properties. In this way, the designer can propose solutions to design specifications and check if those solutions would correspond to specifications according to heuristics before testing them experimentally.

4. Conclusions and perspectives

The article presents Formultools, a tool to support decision-making process for the design of cosmetic emulsions at early stages. Currently, the tool can perform three functions: exploration and selection of ingredients and verification of cosmetic formulations. It was designed to make it as practical as possible which is why it has the form of a mobile application. In a near future, it will be tested with experts and improved for its subsequently application in real design cases.

Formultools was developed in co-design between experts on cosmetic formulation and computer science. Additionally, it was continuously tested with users and iteratively improved. As a result, the tool was developed in a very agile process.

In the long term, the tool will be enhanced to assist the design process in a more holistic way. This will require the implementation of new features to enable information management, learning from each successful design, use by various design agents, among others, while maintaining its simplicity and usability.

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