ECCE AB 21 virtual event
Engineering the Future
20 - 23 September 2021

Towards an ontology-based decision support system for the design of emulsion based cosmetic products

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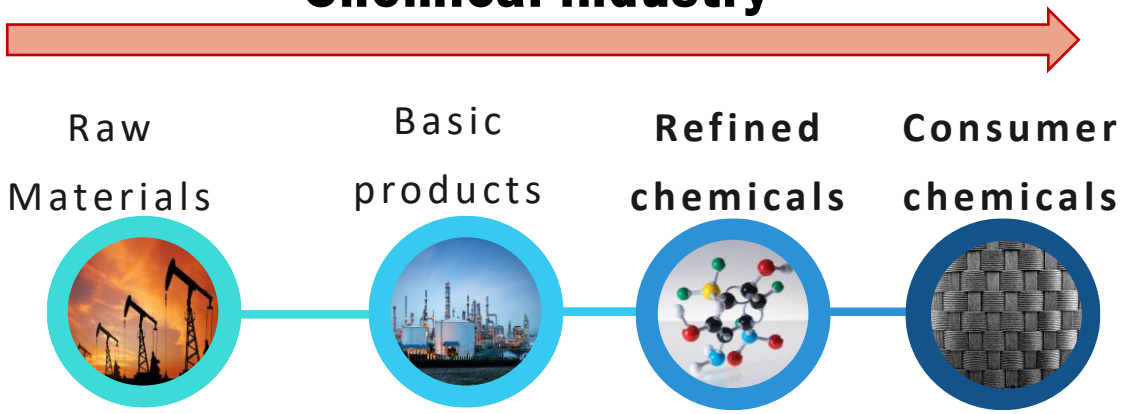
Trends in chemical products engineering

Chemical industry



Process Focus design

- Continues Processes
- High Volume
- Low Cost

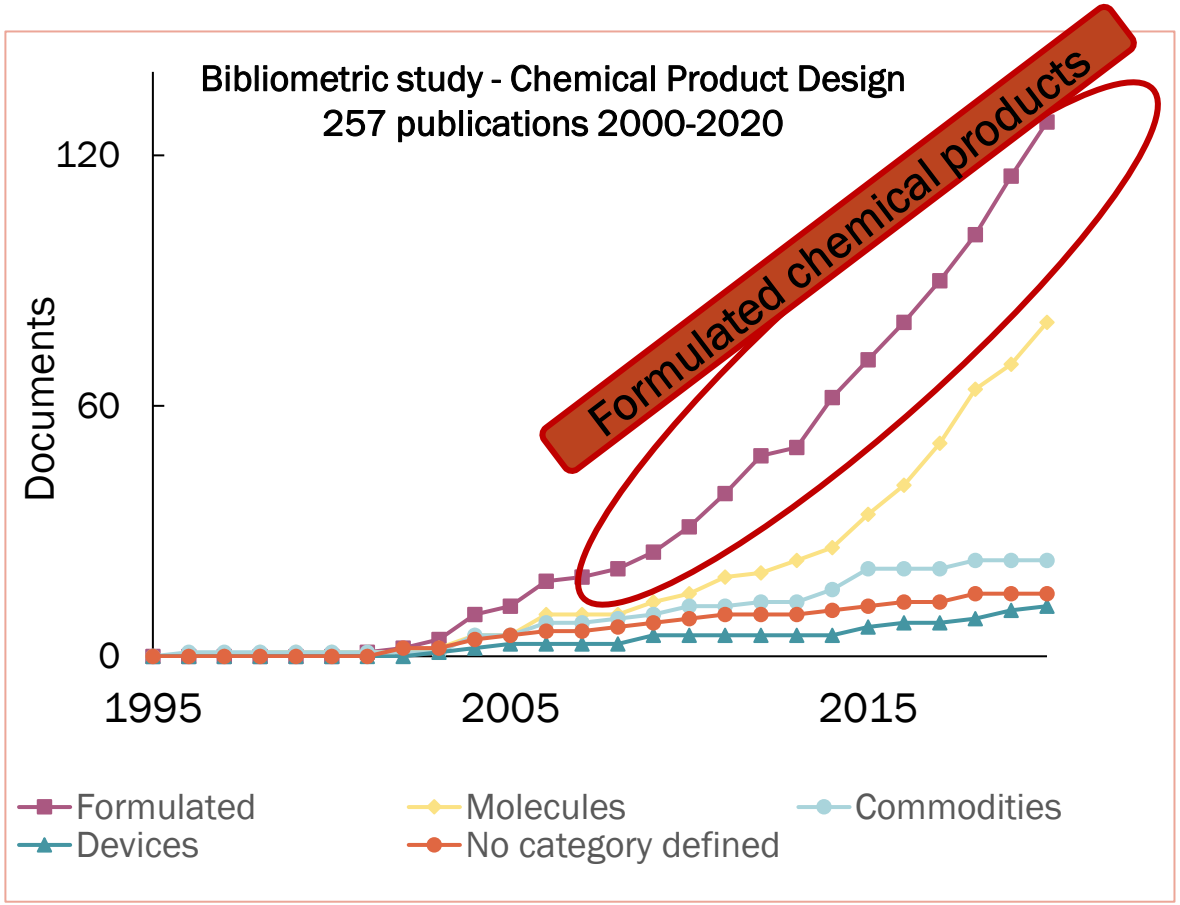
Product Focus design

- Batch Processes
- Low Volume
- High quality

Big Companies

SEMs

Research in Chemical product



Hegedus, L. L. (2005). Chemical engineering research of the future: An industrial perspective. *AIChE Journal*, *51*(7), 1870–1871.

Context

Trends in the chemical industry

Commodities	Produits chimiques de performance	Produits **chimiques spécialisés** et **de consommation**

Produits moléculaires

Volume élevé - Faible coût

Produits formulés

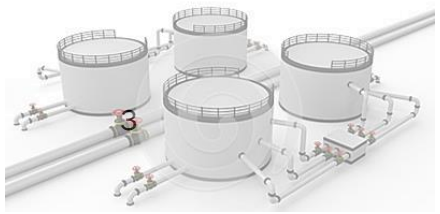
Faible volume - haute qualité

Big Companies

Conception axée sur les procédés

Opportunités pour les PME

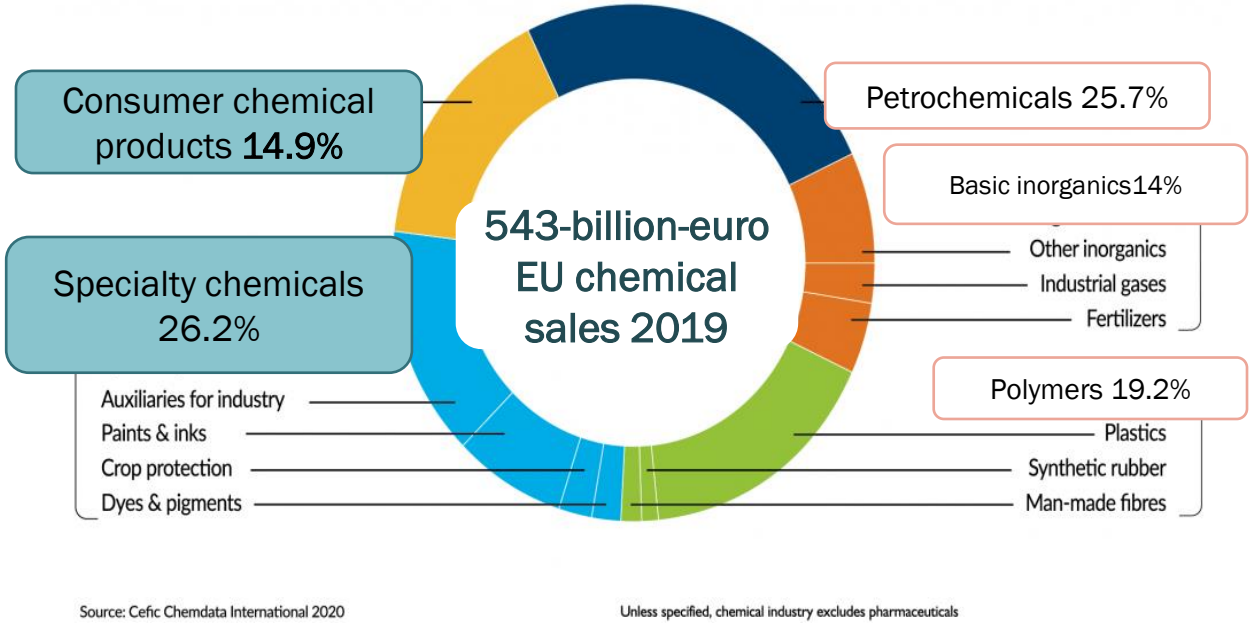
conception axée sur le produit



Some market trends

CHEMICAL SECTOR

European Union chemical sector(1)



Source: Cefic Chemdata International 2020

Unless specified, chemical industry excludes pharmaceuticals

(1) Cefic Facts and Figures 2021

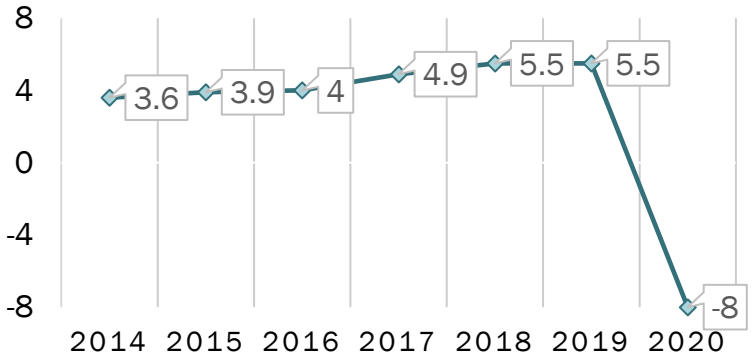
COSMETIC SECTOR

Worldwide cosmetic market

Estimated market 2020 (2)

€200 Bn

Growth of the worldwide cosmetics market over 10 years



Cosmetic sector in France (3)

24 billion €

82% of VSEs and SMEs

(2) https://www.loreal-finance.com/

(3) febea.fr

Comparison: chemical process and product design

COMMODITIES/PROCESS DESIGN

- **Raw materials and chemical routes selection**
- Purity and selectivity
- Process intensification
- Energy integration

FORMULATED PRODUCTS/PRODUCT DESIGN

- From needs to specification
- Ingredient's selection
- **Ingredients-process** synergy
- Scale-up restrictions

1. https://www.icis.com/explore/resources/news/2021/03/12/10617016/eu-chemicals-need-stable-strong-regulatory-framework-to-grow-execs
2. Gani, R., & Ng, K. M. (2015). Product design - Molecules, devices, functional products, and formulated products.

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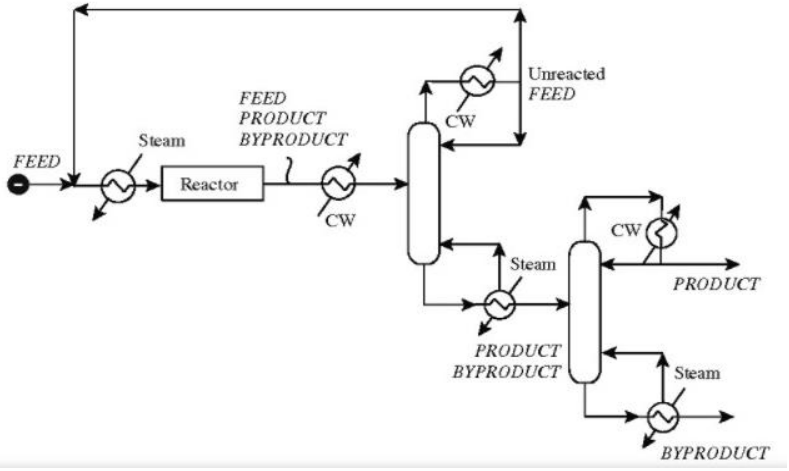
Robust methodology for process design



Unit operations
Thermodynamics
Transport phenomena

Systems thinking

Comparison: chemical process and product design

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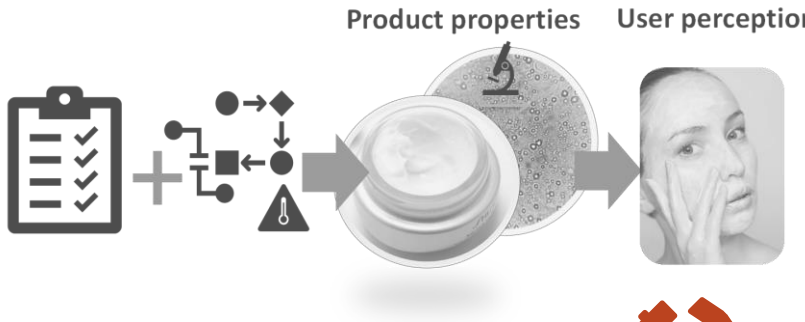
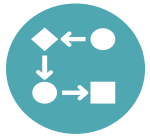


No robust methodology yet

Challenges in the design of formulated products

Challenges during formulation



Complexity. The design process is not sequential but iterative.

Product development is based on Know-how and staff experience.

There are many sources of information, and it is often incomplete

There is a high uncertainty in decisions, especially in early design stages

BtoC. Fuzzy target properties.

NEED Formalization of the design of formulated products and associated data

Ontology : knowledge management approach

Ontology is “an explicit specification of a conceptualization” which is an abstract, simplified view of the world that is represented for some purpose. (1)

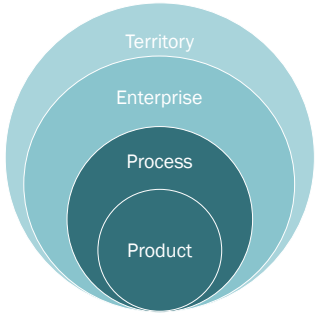
ADVANTAGES

Knowledge representation

Consistent and reliable knowledge representation

Industry 4.0

Knowledge valorization
Digital application



Greater complexity

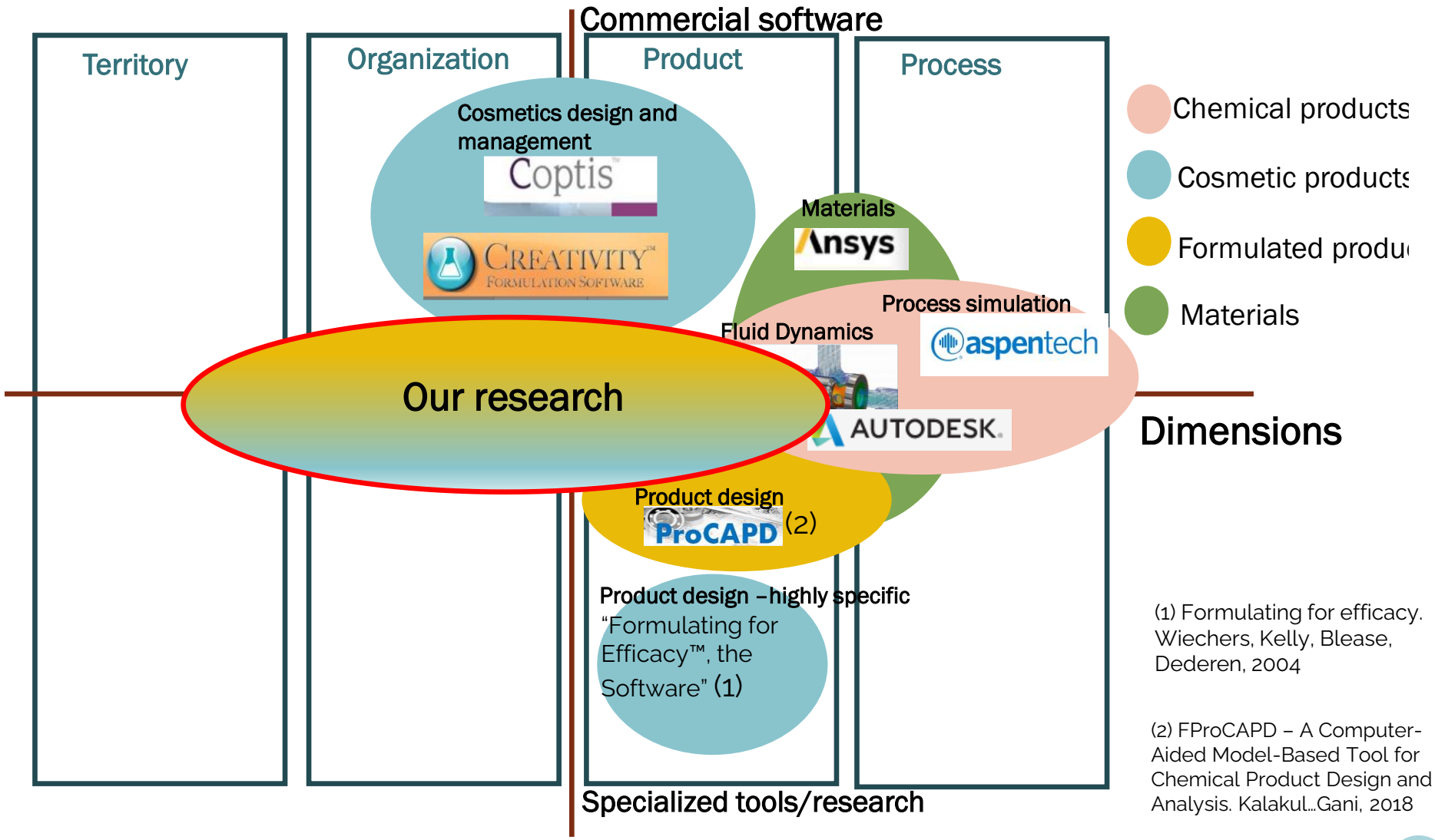
Designer teams, SEM, organizations
Learning from experience

(1) Gabriel et al. 2016

Our research: interdisciplinary and growing

- Formulated products
- Consumer products
- Cosmetic products

- Multi- scale from an organizational point of view/ consideration of the design context.
- Holistic: from need análisis until producto formulation



(1) Formulating for efficacy. Wiechers, Kelly, Blease, Dederen, 2004

(2) FProCAPD – A Computer-Aided Model-Based Tool for Chemical Product Design and Analysis. Kalakul…Gani, 2018

Ontology : knowledge management approach

Ontology is “an explicit specification of a conceptualization” which is an abstract, simplified view of the world that is represented for some purpose [1]

ELEMENTS [2]

Individuals/instances

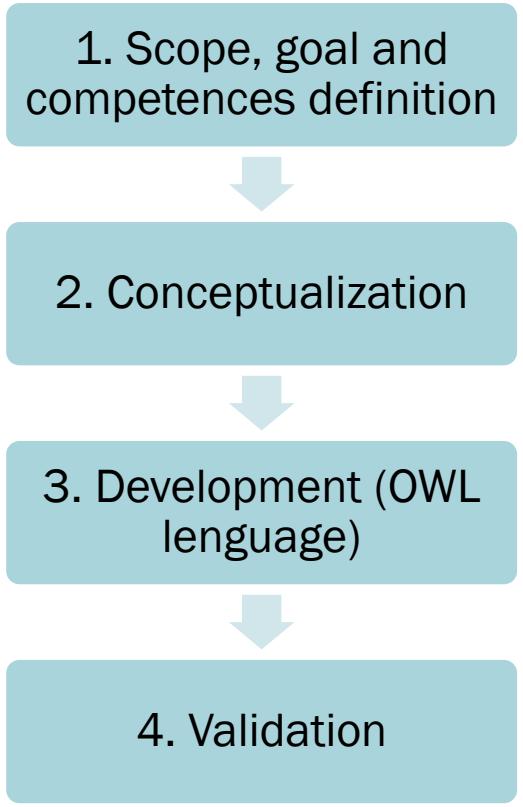
Objects in the domain in which we are interested

Property/slot/attribute

Object properties are relationships between two individuals. Datatype properties describe relationships between individuals and data values.

Class/concepts

Sets containing individuals



[1] Gabriel et al. 2016

[2] Protégé OWL tutorial. University of Manchester

Ontology scope and contextualization

1. Scope, goal and competences definition

The scope of the ontology is the **representation of the information and knowledge developed by our research group in chemical product design** (1) (2). It comprises a flexible design workflow, ingredients and heuristic databases and developed study cases.

The goal is to create a system to assist the decision-making process during formulated product design and more specifically cosmetic product design.

It can be used in a near future for the development of decision support software for the design of formulated products, capable of

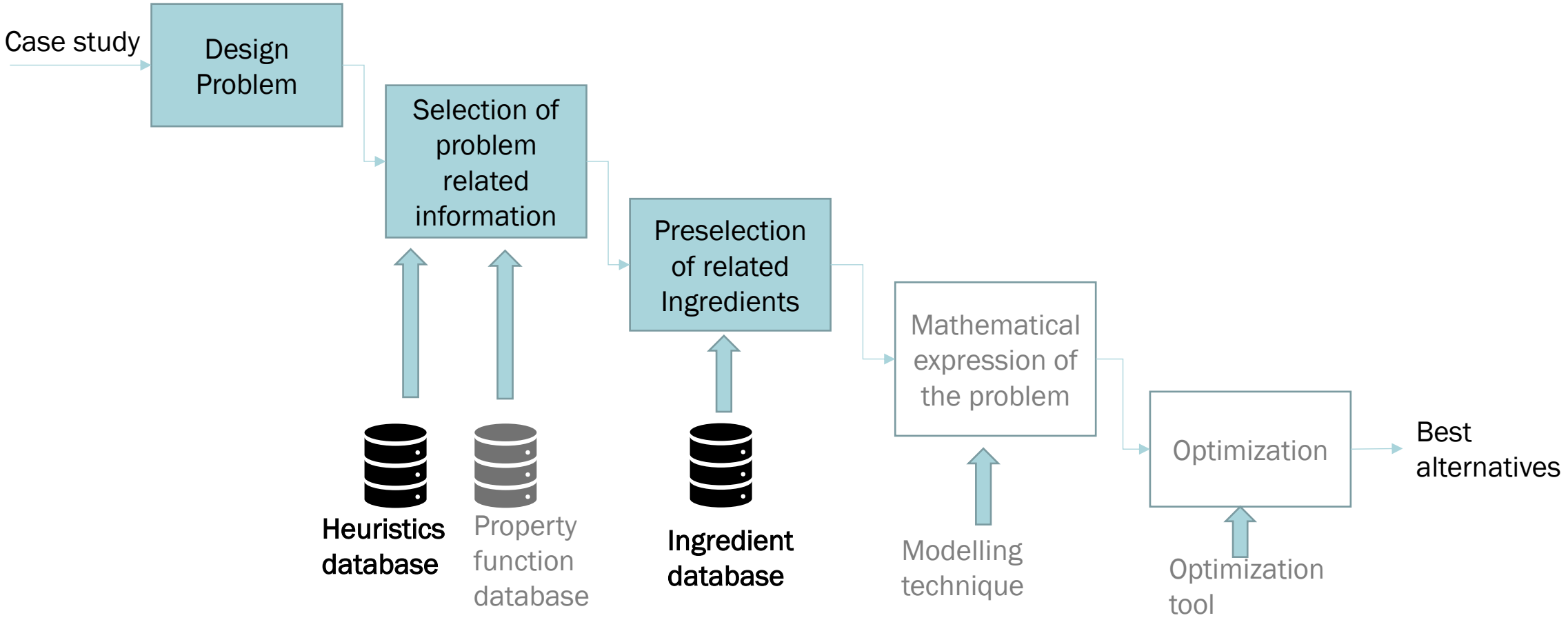
a. Present and graphically represent relevant information based on a query of a user.
b. Store information for specific developed cases
c. Combine heuristic, strategies and ingredient information for decision making or recommendations.

(1) Serna et al. 2021
(2) Arrieta et al. 2019

Ontology scope and contextualization

2. Conceptualization

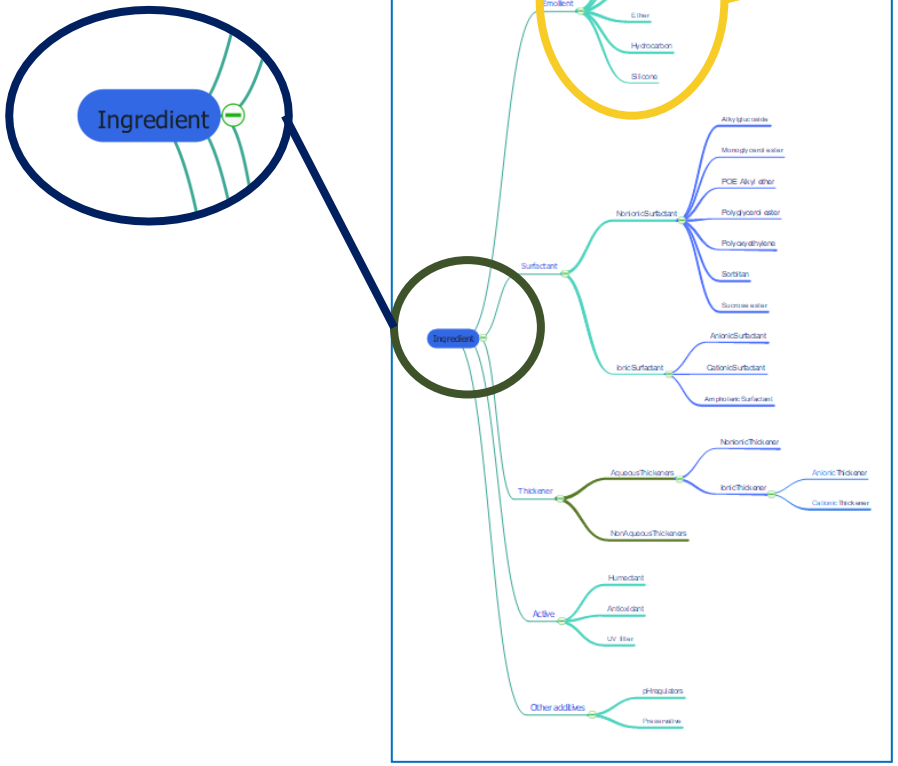
Design process

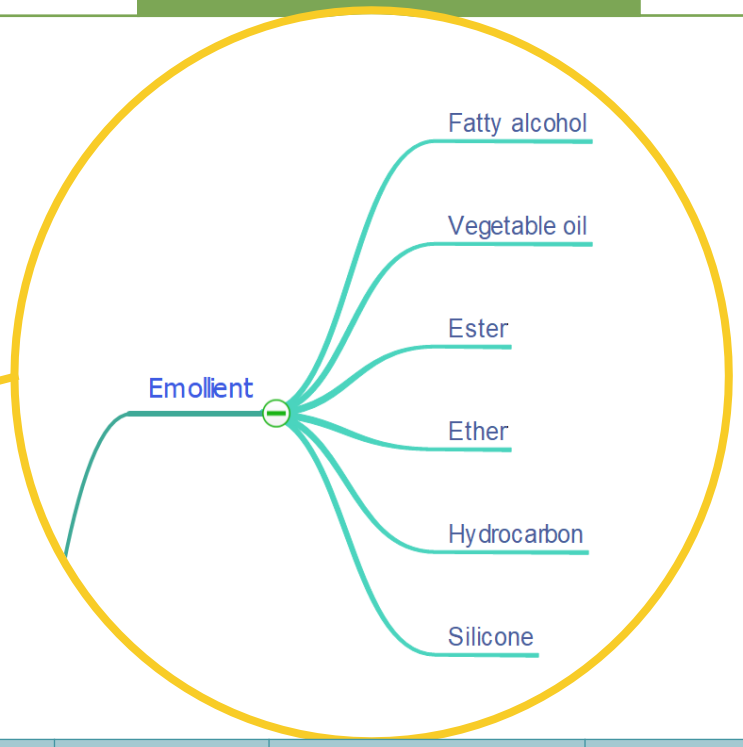


Ontology development

3. Development

Ingredient database





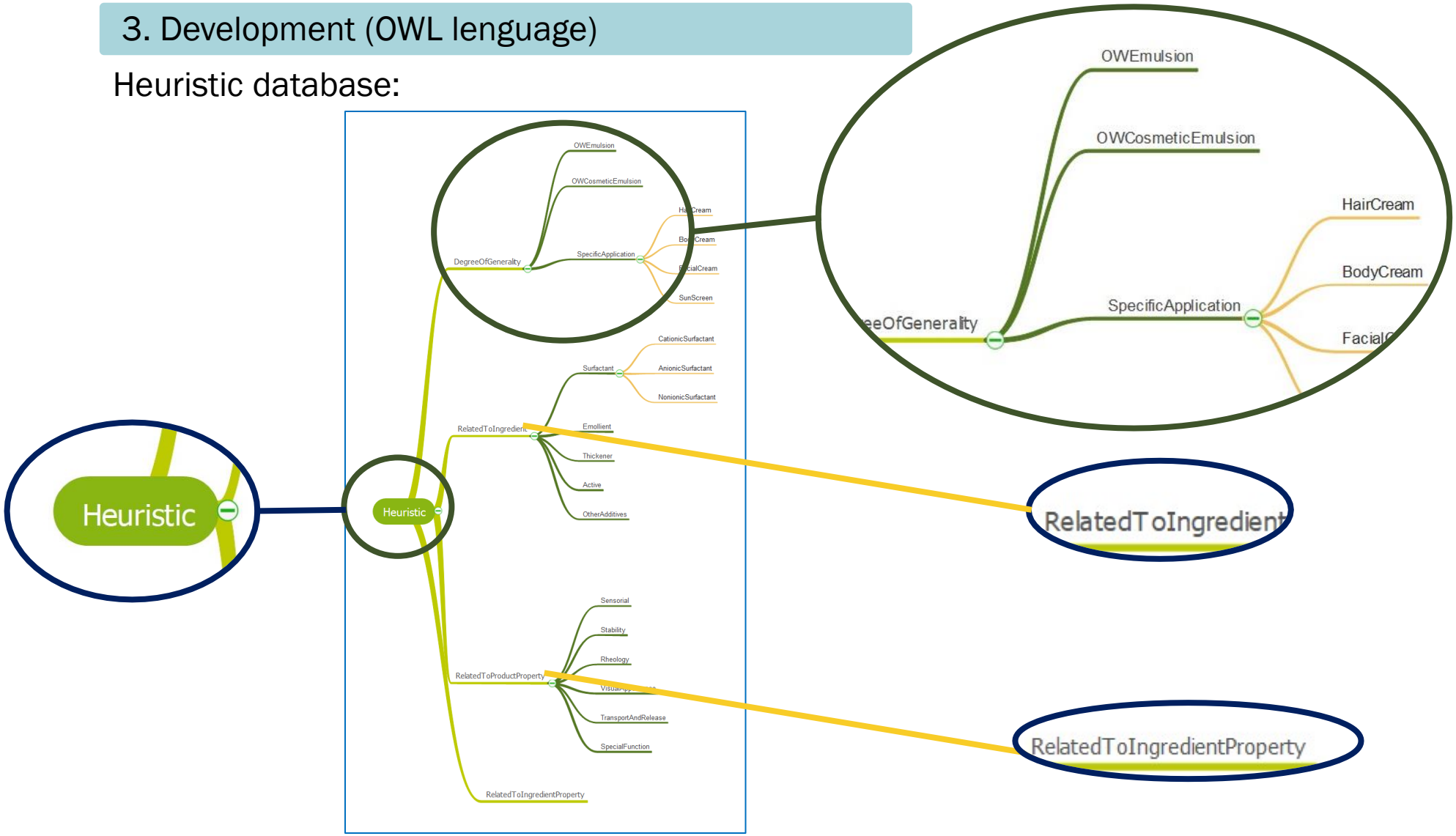
Property	Type	Cardinality	Allowed values	Additional description
Required HLB	Real	single		The Required HLB of the oil is equal to the calculated HLB of the emulsifier system that provides the most stable emulsion
greasiness	String	single	{1-4}	reflects the oiliness of the skin after a lotion is applied
spreading	String	single	{High, Medium to high, Medium, Medium to low, Low}	capacity of a fluid to displace another fluid on a given surface
polarity	String	single	{High, Medium to high, Medium, Medium to low, Low}	related to properties such as the Hansen solubility parameters, KOW, and required HLB.

13 properties for emollients

Ontology development

3. Development (OWL lenguage)

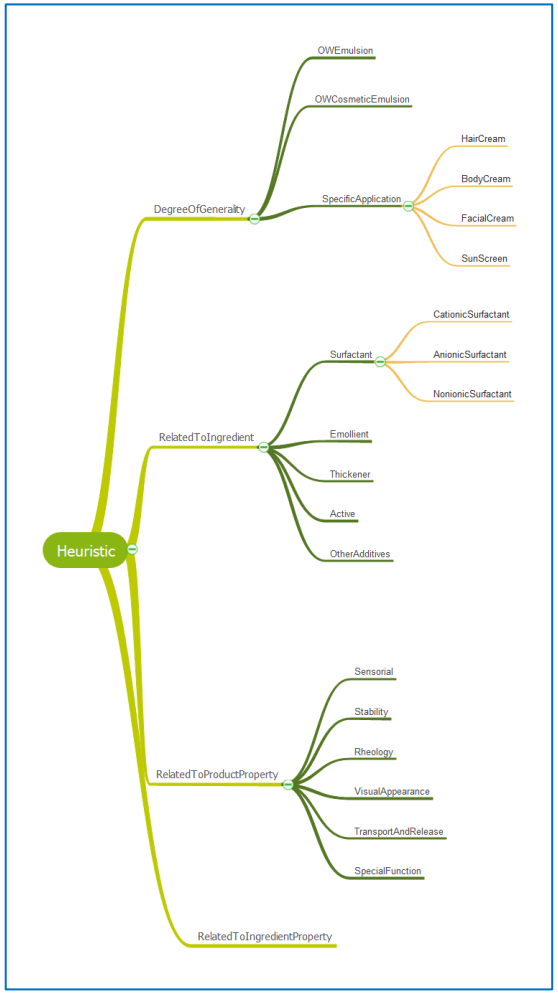
Heuristic database:



Ontology development

3. Development

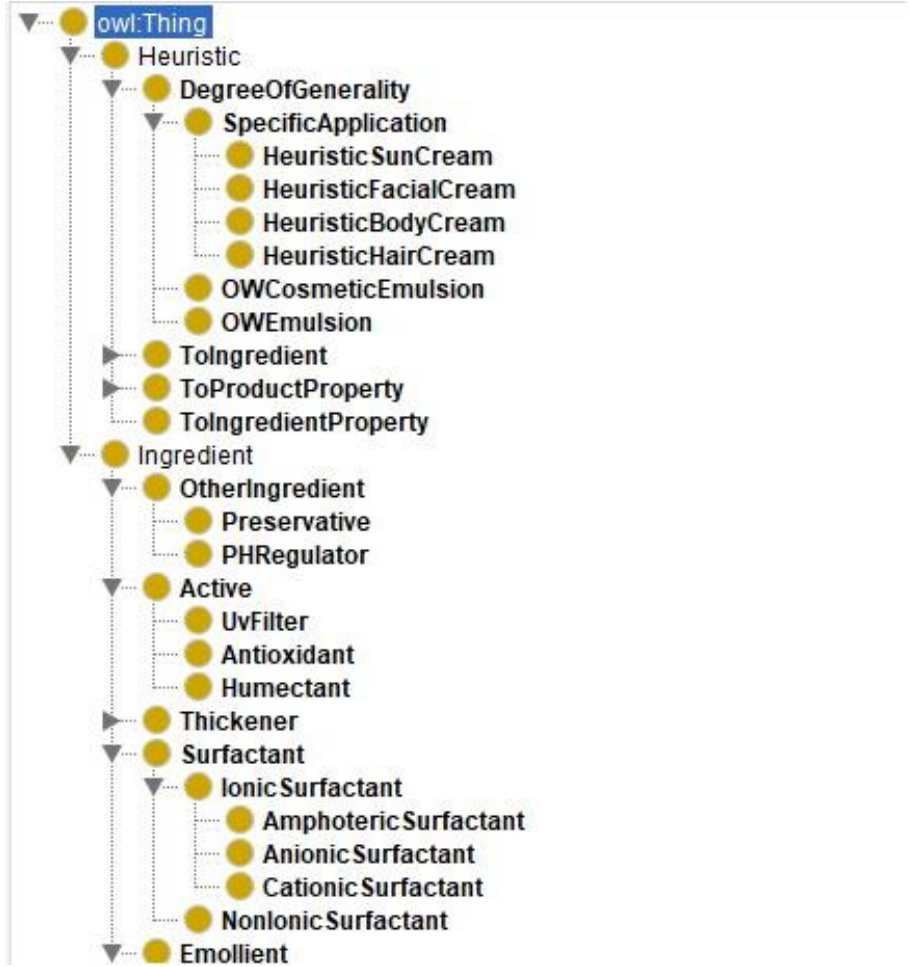
Heuristic database:



Example (instance)	HeuristicType	deegreeOfGenerality	Product Property
Rheology: when not thickener polymer is used, the concentration of fatty alcohol is at least twice the cationic polymer in molar base	Ingredient	SpecificApplication: Hair Cream	RheologicalProfile
Sensorial: at least one emollient of each spreading type should be used: high, medium and low	IngredientProperty: spreading	OWCosmeticEmulsion	Sensorial

Ontology development

3. Development (OWL lenguage)



Ontology example

4. Example of information from both databases

Call all heuristics related to the product hair conditioner

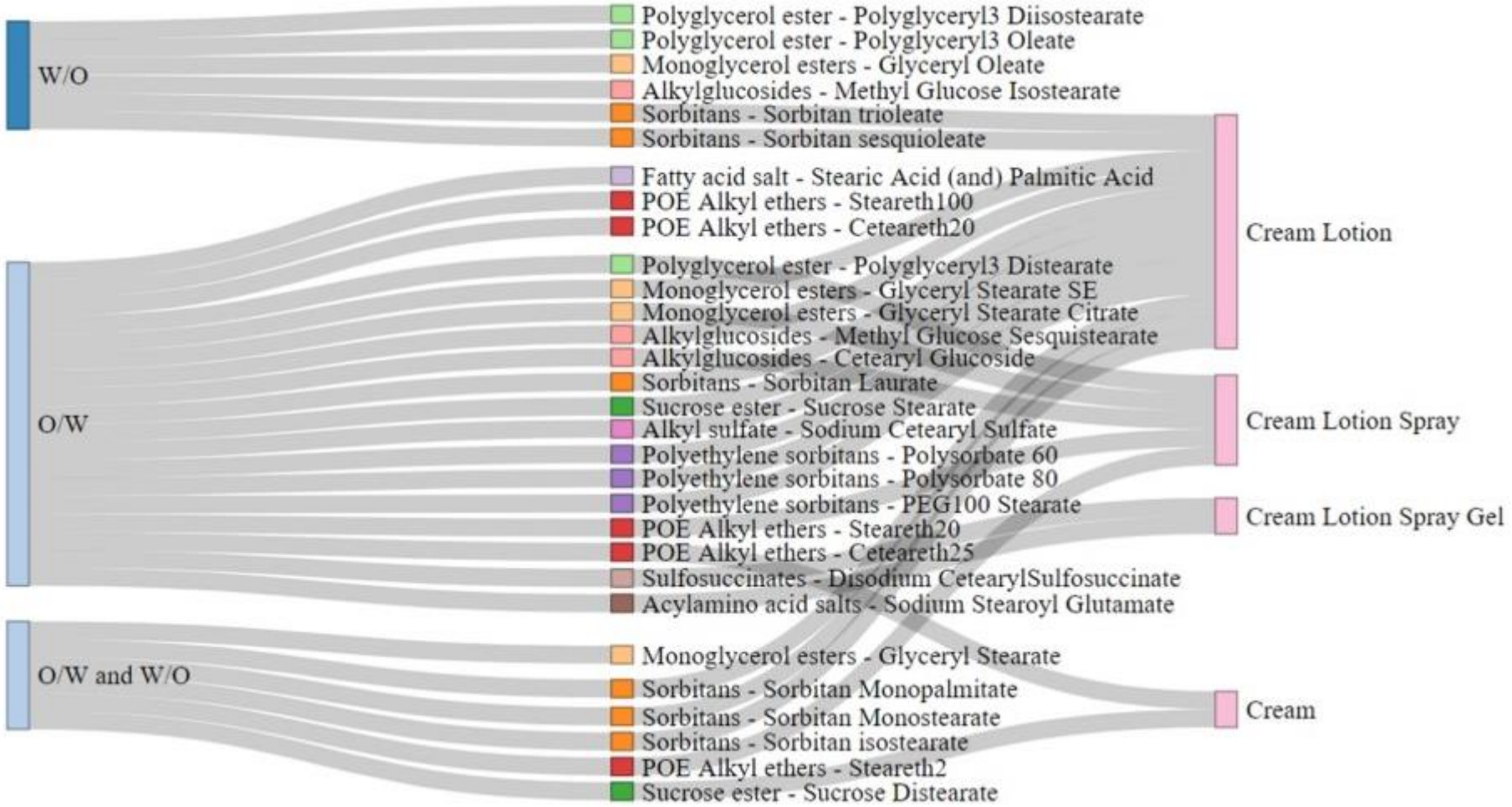
Product	Applicability	Description	Ingredientrelated	Product Characteristic
Hair condicioner	very specific [Hair conditioner]	O/W emulsion with 10 to 25% oily phase	oilyphase%	General
Hair condicioner	very specific [Hair conditioner]	Usually, cationic surfactants are used to control hair static	CationicSurfactant	Sensorial; Functional
Hair condicioner	veryspecific [Hair conditioner]	Combination of cationic surfactants and the sensory characteristics of conditioners	CationicSurfactant [Instance, %]	Sensorial [Moist and lubricating; Moist and soft; Soft and moist]
Hair condicioner	O/W Cosmetic emulsion	Ideal cream should have an “initial” viscosity n1 between 1350 and 3500 Pa.s and a “final” viscosity n2 between 0.023 and 0.500 Pa.s. Also, the “final” viscosity is perceived at a typical shear rate of ~500 s-1	Thickener[Instance, %];oilyphase;equation	Rheology [Rheological profile]
Hair condicioner	veryspecific [Hair conditioner]	when not thickener polymer is used, the concentration of fatty alcohol is at least twice the cationic polymer in molar base	Fattyalcohol, %	Rheology [Rheological profile]
Hair condicioner	O/W Cosmetic emulsion	A typical product specification is a greasiness value in the middle of the scale: between 2.0 and 2.4	Emollient,greasiness,%	Sensorial; greasiness
Hair condicioner	O/W Cosmetic emulsion	Cationic surfactants at about 20% of the oily phase, should stabilize the emulsion	CationicSurfactant, %	Stability
Hair condicioner	O/W Cosmetic emulsion	there should be two but not more than 3 cationic surfactants	CationicSurfactant	General
	O/W Cosmetic emulsion	at least one emollient of each type should be used: high, medium and low	Emollient,spreading, %	Sensorial;spreading

Ontology example

4. Example of information from both databases

Call information and represent it graphically

Class: Surfactant

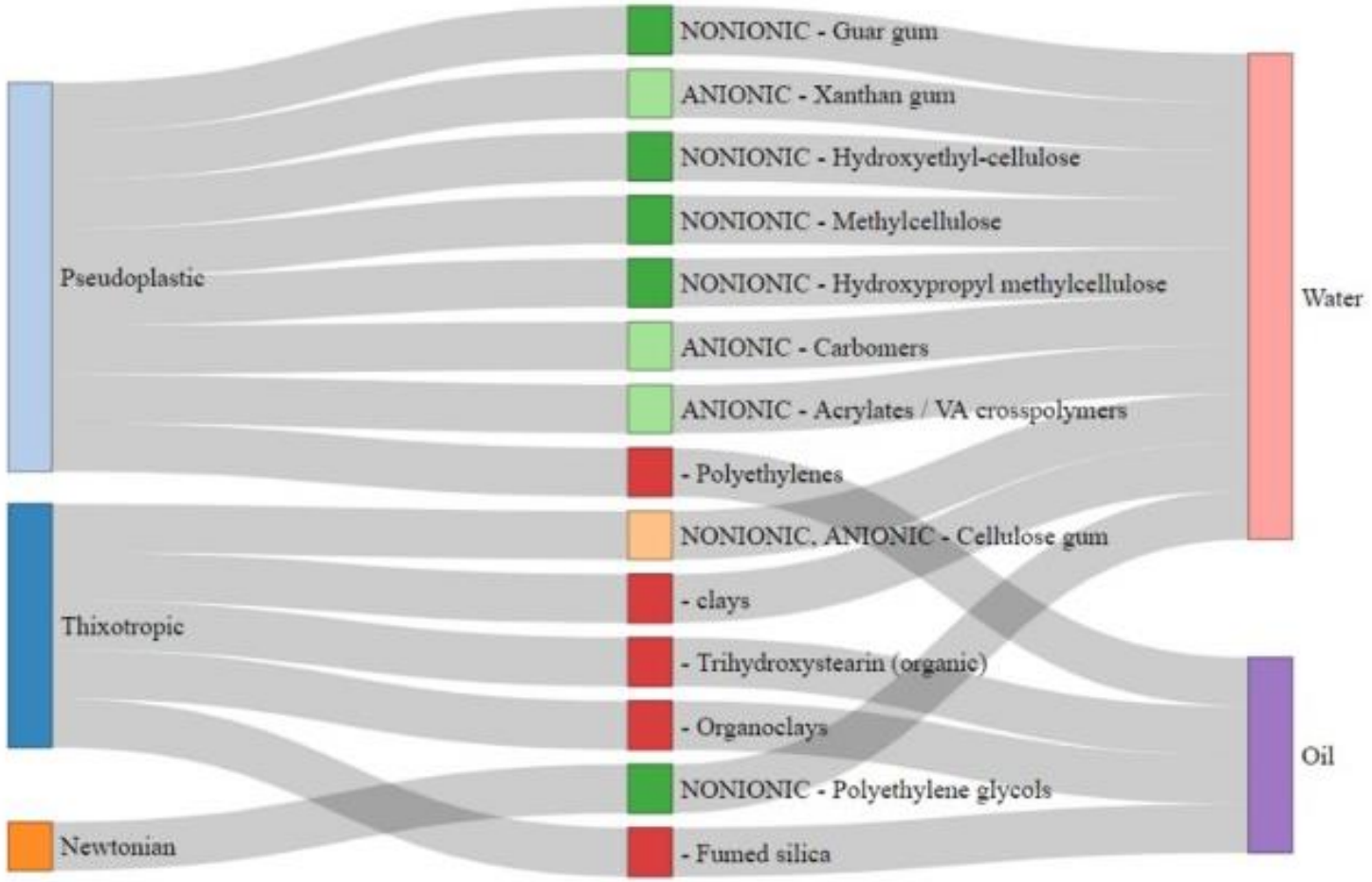


Ontology example

4. Example of information from both databases

Call information and represent it graphically

Class: Thickener



Ontology example

4. Example of information from both databases

Call all ingredients by property

Ex: low spreading

Category	INCIName	Cost (USD/kg)	Greasiness*	RHLB	HLB	Hazard Index	Spreading
Emollient	Cetyl Dimethicone (very high viscosity, nonpolar)	35	3.2			1	Low spreading
Emollient	Dimethicone 1000 CSt	29.3	3.2	5		3	Low spreading
Emollient	Oleyl Erucate	23.9	2			1	Low spreading
Emollient	Persea Gratissima Oil	16.7	2	7		1	Low spreading
Emollient	PPG-14 Butyl Ether	23	3.2			1	Low spreading
Emollient	PPG-15 Stearyl Ether	21.75	2	7		1	Low spreading
Emollient	Triisostearin	30	3.2	8		1	Low spreading

Conclusions

Chemical product design challenges

Complexity. The design process is not sequential but iterative. It is mostly based on expert knowledge

Formalization

It is necessary to structure knowledge and information for the design of formulated products.

Ontology for knowledge management

It is a versatile tool to represent knowledge that can be easily adapted, and expanded

It can be used to create digital applications

It can be used to search and represent specific data

Our Ontology

It represents the knowledge and information for formulated product design and cosmetic product design developed and gathered by our design team

It has been especially used to represent information from ingredient databases and heuristics.

The ontology organizes ingredients according to their functionality and chemical nature and characterizes them with properties relevant to their use in formulations

The ontology organizes ingredients according to their functionality and chemical nature and characterizes them with properties relevant to their use in formulations

The ontology organizes the heuristics according to the desired properties of the product and the ingredients and properties involved

The combined use of the two databases allows for a comprehensive view of the formulation possibilities.

Perspectives

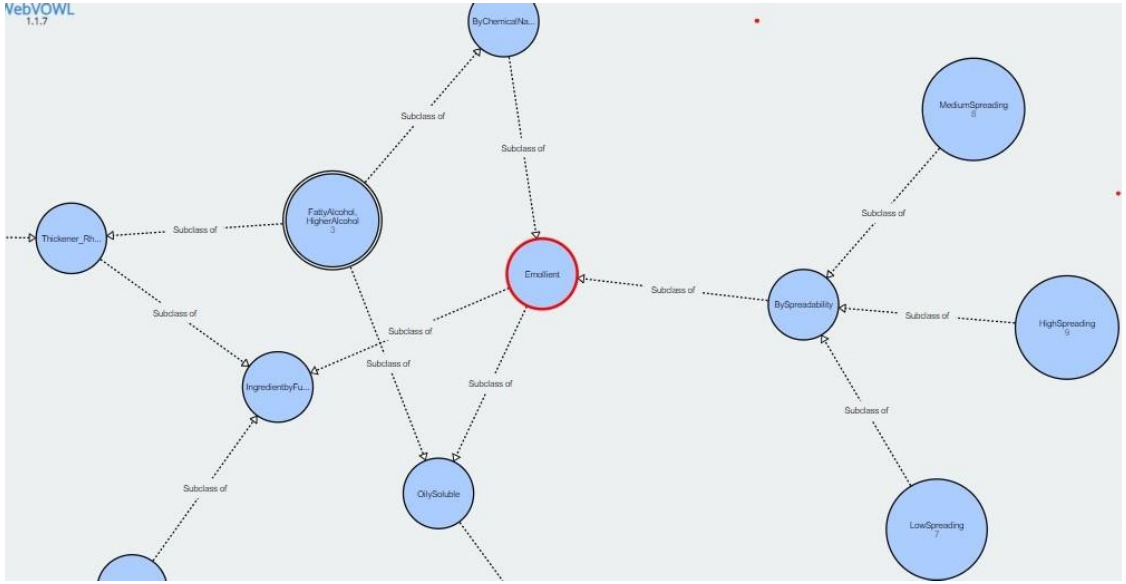


Figure 1 : Ontology – Ingredient data base

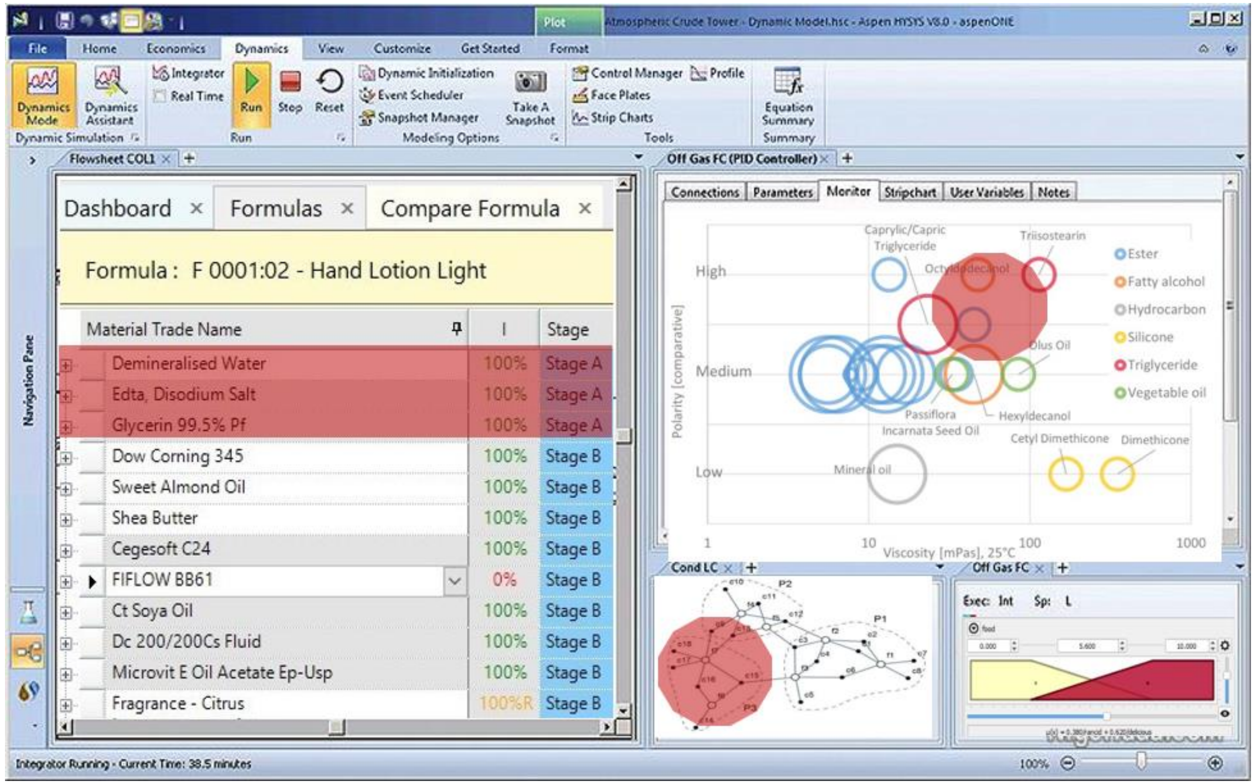


Figure 2 : Layaout of decision support software

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