

Supporting Information

A methodology for emulsion design based on emulsion science and expert knowledge. Part 2: An Application in the Cosmetics Sector

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Selection of ingredients – case study

Table S1. Explanation - Ingredients for a facial moisturizing cream containing calendula oil - case study

Ingredient type		Ingredient	Concentration	Reason	Warnings/recommendations
Oily phase 20%	Emollients/ oils	Caprylic/Capric Triglyceride Isopropyl myristate	6 to 10%	According to ingredient database presented in the first article, these oils give a light sensation and a low oily after-feeling. Other oils have similar properties (within the database from the previous articles it is possible to find more). The availability criterion was also considered for a final decision. They are added in high proportions to ensure the desired final sensation	Proportions can be change during experimentation to have a low oily sensation in the final product
	Oil - natural	Shea butter almond oil	Low concentration <2%	Natural oils are used in low concentrations to avoid rapid product oxidation (as preventing in warnings from Table 5). Almond oil is selected because it has a low oily sensation as expected from product specifications. Shea butter is selected due to its high moisturizing effect (also a requirement) and the product claim of naturalness	
	Fragrance	Lemongrass oil	<0.1%	Fragrance was consulted with a group of customers. Calendula oil is also part of the product fragrance	Attention should be paid to the low resistance of fragrances to high temperature
Surfactants	Surfactant system	System 1: Main surfactant- Polysorbate 80	2.5-3.5%	As presenting in a warning from Table 5, a surfactant system with a relatively high HLB is required to	Except for sucrose palmitate, all surfactants

		+Sorbitan stearate +Glyceryl monostearate System 2: Main surfactant- Sucrose palmitate +Cetearyl glucoside +Glyceryl monostearate System 3: Main surfactant- POE 100 stearate +Sorbitan stearate +Glyceryl monostearate		produce stable O/W emulsion. Considering this and the ingredient database presented in the first article on the methodology, three surfactant systems are selected: - Two surfactant systems based on polyethoxylated (POE) compounds which have a high HLB (over 10) and are relatively inexpensive. Because of availability, a system with polysorbate 80 as main surfactant and another system with POE 100 stearate as main surfactant are selected. Similar systems have been used in similar conditions for cosmetic creams with positive results (Iwata and Shimada, 2013). - A third surfactant system based on sucrose palmitate which is biobased and has a high HLB is selected. This system must be prepared at neutral pH and once the emulsion is formed, pH can be decreased ¹ .	are soluble in the oily phase
-	Rheological modifier/ Thickener	Cetearyl alcohol and cetyl palmitate	2-5%, 3%	These two oily compounds can be used to increase product viscosity up to the expected viscosity according to the design problem. The percentage of use is to be tuned experimentally to achieved the desired rheology and texture ² .	Soluble in the oily phase
Aqueous phase	Rheological modifier (second)	Xanthan gum	0.1-0.2%	Xanthan gum is selected from our database because it has a pseudoplastic behavior (as expected from	Soluble in water,

				Figure 4), it works well at acid pH, and it is naturally derived. It is used at low concentrations 0.1-0.2% because of its high efficiency ³	Dispersible in glycols as glycerin
Acid	citric or lactic acid	Until pH of (4.5-5.7)		Weak acids frequently used in cosmetic	Add after emulsification to adjust the final pH value of the product
Glycol	Glycerin	3%		It is a highly availability and low-cost humectant. It is added to perform the function of hydration. A percentage of 3 was defined based on similar formulations ³	Water soluble
Preservative	Benzyl alcohol and dehydroacetic acid	0.6%		According to our cosmetic preservatives database, for an acid pH it is possible to use preservatives based on phenoxyethanol, benzyl alcohol, benzoic acid, potassium benzoate and parabens. Parabens must be avoided, because they have a negative public image and are contrary to the specification of naturalness. Considering these arguments, and because of its availability, a preservative system based on benzyl alcohol and dehydroacetic acid is used. Concentration is selected by following supplier recommendations.	Soluble in polar solvents such as glycerin, Decrease pH of the emulsion
Antioxidant	Calendula oil Acetate tocopherol			Calendula essential oil is selected because of design specifications. Acetate tocopherol is also added to boom antioxidant action (to achieve antioxidant expected activity)	Low resistance to high temperature

References

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- (3) Iwata, H.; Shimada, K. Formulas, Ingredients and Production of Cosmetics. *Formulas, Ingredients and Production of Cosmetics*. Springer: Tokyo 2013, p 221.