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Heuristic-based computer-aided formulation of ice creams sweetened with jaggery

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To my parents Mary Amoako and James Boahen, who made so many sacrifices for me to be where I am today and gave me the love I needed.

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Resumen

Formulación asistida por computadora basada en heurísticos de helados endulzados con panela

Panela es un endulzante in bruto artesanal obtenido por evaporación abierta de jugos de caña, y es bien conocida por sus propiedades nutricionales y funcionales. La meta de este trabajo es usar un método in sillico para desarrollar formulaciones de helados incorporando panela como substitute parcial o total del azúcar refinado. Por eso, se consultaron a expertos para definir mezclas prototipas conteniendo agua, leche descremada en polvo, crema de leche, vainilla, emulsificantes, aceite de palma y endulzante (solo azúcar o solo panela). El desempeño de los prototipos fue evaluado en términos de densidad, aireado, viscosidad, pH, textura, punto de fusión y velocidad de derretimiento. El resultado fue que el uso de panela no afecta a las propiedades evaluadas. Las heurísticas disponibles, las normas y las propiedades de desempeño objetivas fueron convertidas en ecuaciones y restricciones matemáticas para construir un modelo informático adecuado para el diseño de helados. El modelo se utilizó para desarrollar productos con un costo mínimo mediante una optimización lineal. Se obtuvieron formulaciones asistidas computadora optímales con diferentes contenidos de panela. Se llevó a cabo una evaluación sensorial de los productos y se comprobó que el uso de panela no influye en la percepción sensorial global del producto por parte de los consumidores. Este enfoque heurístico podría adaptarse fácilmente a la formulación asistida por computadora de otros productos alimentarios innovadores.

Palabras claves: Helado, panela, endulzante, diseño de productos, heurísticos, diseño asistido por computadora

Abstract

Heuristic-based computer-aided formulation of ice creams sweetened with jaggery

Jaggery is an unrefined craft sweetener obtained from open evaporation of sugarcane juices, and is well known for its nutritional and functional properties. The aim of this work is to use an in-silico approach to develop ice cream formulations that incorporates jaggery as a partial or total substitute for refined sugar. For this, experts were consulted to define prototype mixtures containing water, skim milk powder, dairy cream, vanilla, emulsifiers, stabilizers, palm oil and sweeteners (only sugar or only jaggery). Prototypes' performance was assessed in terms of density, overrun, viscosity, pH, texture, freezing point and melting rate. It resulted that the use of jaggery does not affect the assessed properties. Available heuristics, regulations, and target performance properties were transformed into equations and mathematical restrictions to build a computer model suitable for ice cream design. The model was used to develop products with a minimum cost via a linear optimization. Optimal computer-based ice cream formulations with different jaggery contents were obtained. A sensory assessment of the products was carried out and proved that the use of jaggery does not influence the overall sensorial perception of the product by the consumers. This heuristic approach might be easily adapted for the computer-aided formulation of several other innovative food products.

Keywords: Ice cream, jaggery, sweetener, product design, heuristics, computer-aided design.

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Lista de symbols and abbreviations

Symbols with Latin letters

Symbol	Term	SI Units	Definition
A	Content of sugar	% wt.	
C_s	Concentration of the sugars' concentration in sucrose equivalence	% wt.	Eq. 1.2
D	Content of dairy product	% wt.	
E,S	Emulsifier-stabilizer	% wt.	
F	Fat content	% wt.	Eq. 1.1
FDP	Freezing point depression	°C	Eq. 1.3
Ing	Content of ingredient	% wt.	
invd	Inverse of the density	$L \cdot kg^{-1}$	
L	Lactose content	% wt.	
LO	Liquid oil proportion between 4 and 5°C	% wt	Eq. 2.2
m	Mass	kg	
MF	Milk fats content	% wt.	Eq. 2.3
MSNF	Milk-solids-non-fat content	% wt.	Eq. 2.6
O	Content of oil	% wt.	
OR	Overrun	%	Eq. 1.4
P	Protein content	% wt.	Eq. 2.5
S	Mineral salts content	% wt.	
SE	Sucrose equivalent	%	Eq. 1.1
TS	Total solids content	% wt.	Eq. 2.1

Symbol	Term	SI Units	Definition
V	Volume	m^3	
W	Water content	% wt.	
WS	Whey solids content	% wt.	

Symbols with Greek letters

Symbol	Term	SI Units	Definition
$\dot{\gamma}$	Shear rate	s^{-1}	
η	Dynamic viscosity	Pa·s	
κ	Consistency	Pa·s^n	
λ	Ratio between air and mix viscosity	1	$\frac{\eta_{air}}{\eta_m}$
ρ	Density		
ϕ	Volume fraction of air	1	$\frac{V_{ic}-V_m}{V_{ic}}$

Subscript

Subscript	Term
DE	Dry extract
i	Variable of summation
ic	Ice cream
m	Mix
req	Required
tot	Total
∞	Infinite

Exponent

Exponent	**Term**
n	Exponent

Abbreviations

Abbreviations	**Term**
DSC	Differential scanning calorimetry
GB	Gigabytes
PCA	Principal component analysis
RAM	Random access memory

Introduction

Non-centrifugal cane sugar (NCS), also known as jaggery, is an unrefined solid sweetener obtained from the open evaporation of sugar cane juices. The thermal treatment that is carried in its manufacturing process confers distinctive organoleptic characteristics to the product, such as a caramel-like flavor and aroma (García et al., 2017). Jaggery is traditionally well-known for being a readily-available energy source in the form of carbohydrates (mainly sucrose), and it is considered wholesome compared to refined or raw sugar due to its higher content of minerals, polyphenols, antioxidants and vitamins (Gartaula & Bhattari, 2014; Alarcón et al., 2021). Jaggery consumption is widely spread in Asia, Latin America, the Caribbean and Africa, and despite being the second largest producer after India, Colombia has the largest per capita apparent consumption with 20kg/yr./person (Alarcón et al., 2020).

Historically in Colombia, the jaggery sector is a cultural heritage, and the product is directly consumed as part of hot or cold beverages and infusions, as a sweetener for coffee, and as a food ingredient. Nevertheless, jaggery consumption has been in decline due to the accessibility to other lower-calorie (e.g. Aspartame, Acesulfame-K, Saccharin, Sucralose, Neotame) and/or commodity sweeteners (e.g. refined sugar). This represents a major threat to the sustainability of the whole Jaggery business in the country, which might jeopardize nearly 300000 rural jobs, corresponding to 12% of the Colombian economically active agricultural population (Min. Agricultura, 2019). In order to boost this economic sector, jaggery could be oriented as an ingredient in industrial food products such as ice creams, where it can enhance the nutritional value and improve the sensory profile.

Similar to the global trends, the ice cream demand in Colombia is steadily increasing and there is an ongoing tendency for premiumization (Euromonitor, 2020). Likewise, there is a growing preference for the consumption of ice creams that contain natural and minimally-processed ingredients, which has driven the growth of the artisanal ice cream sector. Taking into account the nutritional characteristics of jaggery, as well as its sweetening nature, there is a potential for its inclusion in frozen desserts belonging to this niche. At this point it is important to assess the impact of jaggery on the performance properties of ice cream. The understanding of these impacts is paramount to develop product design strategies, mainly when using computer-aided approaches.

Traditionally, food product design is carried out by experts using trial and error methodologies. Once the product is designed and engineered, prototypes are made until designer expectations are fulfilled. Then, the selected prototype is subjected to consumer assessment for sensory analysis and feedback, which is used for adjustment or further development. Eventually, the selected formulation is released to scale up at the industrial level. All this process is highly resource-intensive and takes long time, thus preventing a rapid product launching into the market. This is a major issue nowadays considering that the global food industry is increasingly pushed to reformulate a large fraction of its products. This is a result of the change in consumer preferences, safety concerns, food labeling regulations, and/or ingredient-based taxing, among other drivers. Alternatively, and as a way to accelerate product development or reformulation mainly when using novel ingredients (e.g. jaggery), the computational design could play a key role (Constantinou et al., 1996). Computational tools are increasingly used in the design and formulation of mixtures and structured products such as cosmetics, personal care and household products, emulsions, and also foods. (Costa et al., 2006; Hill, 2009)

Among the different computer-aided approaches for product conception, recent developments have enabled the accelerated design and engineering of products using integrated methodologies. Particularly, the combination of expert knowledge, computer modeling and experimental validation has enabled a rapid and successful design of emulsified products (Arrieta-Escobar, 2018). By means of this approach, consumer preferences, performance properties, and formulation heuristics are translated and systematized into mathematical models that can be further programmed for the optimization of the products. As the models can involve a large set of continuous and discrete variables of nonlinear nature, together with a large number of restrictions, the solution of the design problem is generally carried out by computer-aided tools. In this case, the design problem can be focused on optimizing the expected performance, reducing manufacturing costs, or enhancing any other objective function. This type of approach seems suitable for the development of novel food formulations including those for ice cream production.

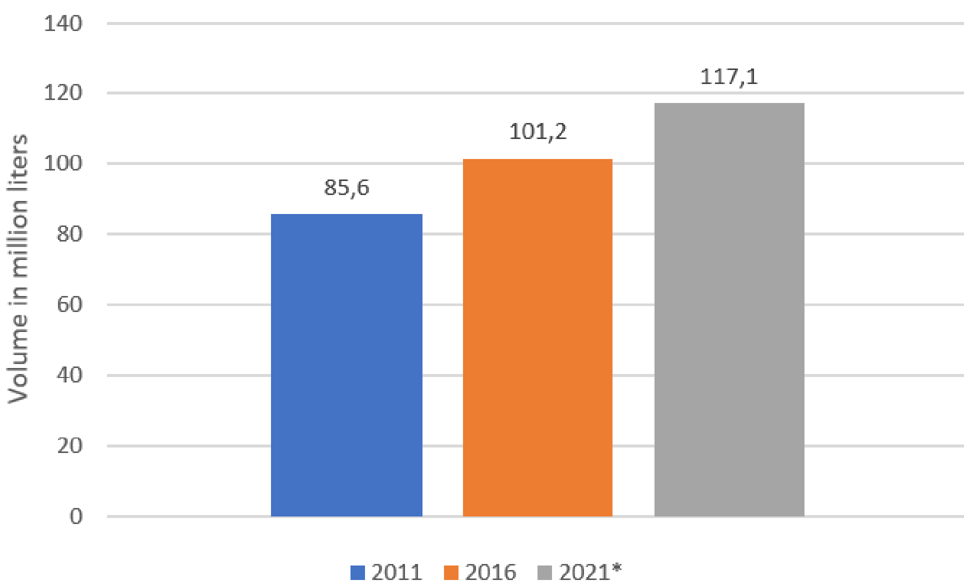
Specifically, in the design of ice creams, different studies have focused on investigating and evaluating the use of alternative sweeteners on formulations including date syrup (Hashim & Al Shamsi, 2016), and agave fructans (Pintor Jardines et al., 2020). However, no reports have been done on the incorporation of jaggery as a sugar substitute. Besides, there are no reports on the computer-assisted design of ice creams. In this regard, this project aims to use the principles of computational design in order to incorporate jaggery as a functional ingredient of ice cream formulations. The study involved the identification of formulation heuristics and restrictions, as well as the determination of quality performance properties of ice cream. These are implemented in a computer model that was optimized to minimize total ingredients' costs. Experiments were also carried out to assess the impact of jaggery on the properties of the product and to verify the suitability of the optimized computer formulation. A final sensory analysis was also performed for consumer assessment and for a final validation of the proposed approach.

1. Ice cream

1.1 Ice cream in Colombia

In Colombia, the ice cream and frozen dessert industry reported sales of nearly COP $1.5 billion in 2019, with an ongoing trend for premiumization (Euromonitor, 2020). Likewise, there is a growing preference for the consumption of ice creams that contain natural and minimally-processed ingredients. These include exotic fruits and special mixed flavors, natural sweeteners, biobased preservatives, all prepared under craft practices. As a result, this has driven a larger growth of the artisanal ice cream segment which could use be a potential jaggery user. The annual consumption of ice cream per capita in Colombia was 3.1 liters/person (Portafolio, 2019), and has been increasing during the last ten years (Statista 2021) as presented in Figure 1-1.

Figure 1-1 Annual sales volume of ice cream in Colombia in 2011, 2016 and forecast to 2021

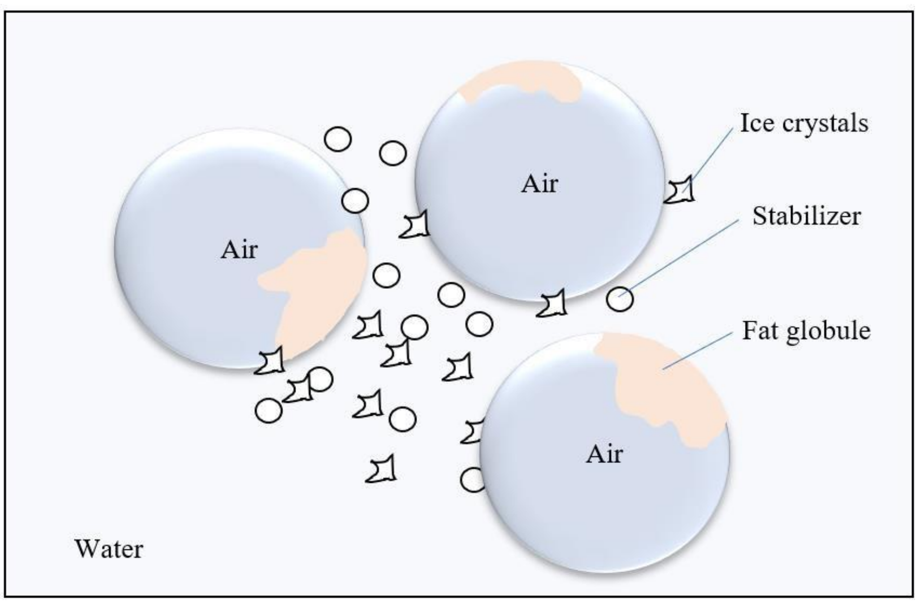


Source : (Statista, 2021)

1.2 Nature of ice cream

Ice cream is a frozen dairy dessert characterized by containing milk solids (but not necessarily milk fats) (Goff, Hartel, 2003). It is an aerated, solidified oil-in-water emulsion, that constitutes a four-phased product (gas phase, aqueous phase, oil phase and solid phase). As a result of this complex microstructure, it is a soft viscoelastic solid that requires a strict formulation and suitable manufacturing process to provide mechanical and thermal stability and to guarantee its physicochemical and sensory properties. The schematic structure of ice cream is described in Figure 1-2. As depicted, the air bubbles are stabilized by the fat globules surrounding them; the bubbles allow the system to be light while the globules ensure a suitable viscosity. The aqueous matrix surrounding the globules represents the most important part of the ice cream, containing water, sweeteners, flavoring, coloring agents, emulsifiers, and stabilizers. Part of the water is in the form of ice crystals which number, shape, and size significantly affect the ice cream’s viscosity, elasticity and mouthfeel, among other properties. The composition of the liquid and solid phases significantly affects the structure of ice cream and therefore must be carefully controlled (Boutonnier, 2018). It is important to underline that the ice cream’s properties depend also on the manufacturing process conditions. In general, in the ice cream industry jargon, the combination of the oil and water phases is referred to as “the mix” (Chavez Montes, 2002).

Figure 1-2 : Ice cream structure (adapted from Boutonnier, 2018)



1.3 Composition

The overall composition of an ice cream differs from one to another depending on the local regulations and on the corresponding product category (i.e. economy, standard, premium, superpremium). For instance, the higher the product's quality, the higher the content of solids and fats and the lower its air content (Goff, Hartel, 2003). The typical ranges of the composition of the different ingredients in the different types of ice creams are listed in Table 1-1.

Table 1-1. Average values of fat and total solids contents, overrun and cost level amongst the most typical ice cream categories (Goff, Hartel, 2003)

Component	Economy	Standard	Premium	Superpremium
Fat	Legal minimum usually 8-10%	10-12%	12-15%	15-18%
Total solids	Legal minimum usually 35-36%	36-38%	38-40%	>40%
Overrun	Legal maximum	100-120%	60-90%	25-50%
Cost	Low	Average	Higher than average	High

Besides fulfilling regulations, a defined set of ingredients and certain formulation rules are required to obtain the desired physicochemical properties to the final product (e.g. density, viscosity, overrun, freezing point, etc.) as well as the sensory characteristics (e.g. color, taste, texture, etc.). In general, and based upon formulators experience, there is an established range of concentrations for the most typical ingredients used in ice creams to avoid undesired characteristics or bad quality of the final product. As observed in Table 1-2, there are typical composition ranges for the most important ingredients namely fat, solids, sweeteners, stabilizers, and emulsifiers, and the mix is completed with water.

Table 1-2. Suggested proportions for hard-frozen ice cream products (Goff, Hartel, 2003)

	Composition (%)						
Milk fat	10.0	11.0	12.0	13.0	14.0	15.0	16.0
Milk solids-non-fat	11.0	11.0	10.5	10.5	10.0	10.0	9.5
Sucrose	10.0	10.0	12.0	14.0	14.0	15.0	16.0
Corn syrup solids	5.0	5.0	4.0	3.0	2.0	-	-
Stabilizer[a]	0.35	0.35	0.30	0.30	0.25	0.20	0.15
Emulsifier[a]	0.15	0.15	0.15	0.12	0.10	0.10	-
Total solids	36.5	37.5	38.95	40.92	40.35	40.3	41.65

[a] Highly variable depending on type; manufacturers recommendations are usually followed

As presented in Table 1-3, each one of the ingredients of ice cream has its own function and provides certain characteristics to the final product. In general, they are gathered in groups, namely: milk fats, milk-solids-not-fat (MSNF), sweeteners (usually sucrose and corn syrup solids), stabilizers, and emulsifiers (Goff, Hartel, 2003). Examples of each category and other optional ingredients commonly used in the mix preparation are listed in Table 1-4.

Table 1-3: Function and limitations of selected ice cream constituents (Goff, Hartel, 2003)

Constituent	Functions	Limitations
Milk fat	Increases richness of flavor Lubricates and insulates the mouth	Relatively high cost and smoothness of texture Hinders whipping May limit consumption due to high calories and satiating effect
Nondairy fat	Provides good structure and texture at lower cost than milk fat, if appropriate solid fat content	Contributes little to flavor and may impart of off-flavor May contribute to greasy texture
Milk solids-non-fat; milk/whey protein concentrates	Improves body and texture (protein) through emulsification and water holding capacity Promotes development of overrun	High amount may cause cooked or salty flavor Potential for sandiness (lactose crystallization) at high concentration
Whey solids	Less expensive than conventional sources of MSNF	High amount of lactose causes freezing point depression Potential for sandiness greater than for conventional sources of MSNF
Sugar	Lowers freezing point Imparts sweetness to the ice cream Improves flavor/texture	Excess sweetness possible Lower hardening temperature needed Ice cream is softer, affecting scooping and the potential for greater recrystallization
Corn syrup solids	Lower cost than sugar Improve body and texture Increases stability of the ice cream	Impart off flavor and chewy texture when overused
Stabilizers	Enhance smooth texture Provide body Enhance shelf life	Excess chewiness may occur Increase melt resistance
Egg yolk solids	Improve whipping ability Impart custard flavor	Foamy melted product Egg flavor may be undesirable
Emulsifiers	Promote fat destabilization, leading to dryness, smoothness, and good melting properties	Increase potential for churning of fat
Total solids (TS)	Smoother texture Firmer body High nutriment content Lessen excess coldness	Heavy, soggy or sticky body Reduce coldness
Flavoring	Increases acceptability	Intensities and harshness may be unacceptable

Coloring	Improves attractiveness Aids flavor identification	Allergic reactions of some people to yellow no. 5 or no. 6 Some consumers dislike added colors

Table 1-4. Essential and optional ingredients for frozen dairy dessert mixes (Goff, Hartel, 2003)

Dairy fat Cream Plastic cream Butter Anhydrous milk fat/butter oil ***Nondairy fat*** Palm oil Palm kernel oil Coconut oil Other safe and suitable vegetable oils ***Milk solids-non-fat*** Concentrated (condensed/evaporated) milk Sweetened condensed milk Milk powder, skim or whole Sweet cream buttermilk, concentrated or dried Whey, concentrated or dried Milk protein concentrates Whey protein concentrates or isolates Hydrolyzed or modified milk proteins Sodium caseinate ***Sweetening ingredients*** Sucrose ("sugar"), cane or beet Invert sugar Corn (or other starch hydrolysates) syrup, varying DE, liquid, or dried High maltose syrup, liquid or dried Fructose or high fructose syrup, liquid or dried Maltodextrin Dextrose Maple syrup, maple sugar Honey Brown sugar Sugar alcohols, e.g., maltitol, sorbitol	***Water*** Potable water Milk: whole, partly skimmed, or skim Cream Condensed milks Liquid sweeteners ***Stabilizers, thickeners*** Sodium carboxymethyl cellulose (cellulose gum), guar gum, locust bean gum, sodium alginate, propylene glycol alginate, xanthan, carrageenan, modified starches, microcrystalline cellulose (cellulose gel), gelatin, calcium sulfate, propylene glycol monostearate or other monoesters, others ***Emulsifiers*** Mono- and diglycerides, distilled monoglycerides (saturated or unsaturated), polyoxyethylene sorbitan monostearate, (60) or monooleate (80), others ***Egg products*** Whole egg: liquid, dried, frozen Yolk: Liquid, dried, frozen ***Salts*** Sodium chloride Sodium salts of citric acid Phosphates—disodium, tetrasodium or, hexameta forms (~0.1% of product) Ca or Mg oxides or $Ca(OH)_2$ ***Flavoring*** Natural or artificial flavors ***Coloring*** Natural or artificial colors

High-intensity sweeteners, E.G., sucralose, aspartame, acesulfame K, stevia

1.4 Sweeteners and jaggery

Among the large variety of ingredients used in ice cream formulations, sweeteners are of major importance. Besides providing a sweet flavor and being an energy source, these compounds also help to develop the characteristic microstructure of ice cream by modifying its physicochemical properties (e.g. solids content, melting point, viscosity, crystallinity, etc.) (Chavez Montes, 2002). Most typical sweeteners were listed in Table 4, and these include natural saccharides (e.g. sucrose from sugar cane or beetroot, sugar honeys, maple syrup, bee honey), synthetic bioderived saccharides (e.g. glucose, fructose or maltose syrups from hydrolyzed starches, dextrins, dextrose, etc.), synthetic alcohols (e.g. sorbitol, xylitol, mannitol), and synthetic high-intensity non-caloric ones (e.g. sucralose, aspartame, acesulfame K) (Goff, Hartel, 2003).

Nowadays, consumers' preferences are focused on minimally processed foods, containing natural ingredients, reduced in refined sugar, salt, and saturated fats, and with valuable functional properties. In this regard, jaggery appears as a potential substitute for refined sugar considering that the sugar profile is similar, but as a whole food, it also contains minerals, antioxidants, polyphenols, flavonoids, and vitamins (Jaffe, 2015; Garcia et al 2017). Table 1-5 lists the minimum mandatory specifications and composition of Colombian jaggeries (ICONTEC, 2009).

Table 1-5. Physicochemical requirements for jaggery (ICONTEC, 2009)

Property	Block jaggery	Granulated jaggery
Moisture (% wt.)	9	5
Ashes (% wt.)	0.8	1
Total sugars - Sucrose (% wt.)	83	93
Total reducing sugars – glucose (% wt.)	5.5	5
Proteins (% wt.)	0.2	0.2
K (mg/100 g)	100	100
Ca (mg/100 g)	10	10
P (mg/100 g)	5	5
Fe (mg/100 g)	1.5	1.5
Colorant	Absent	Absent

Jaggery is produced by open evaporation of sugar cane juices, and as a result of this thermal treatment, it has a characteristic caramel-like flavor and aroma (García et al., 2017) that can improve the sensory profile in some types of ice creams. In 2019, the jaggery subsector was the second largest agroindustry in Colombia in terms of social importance, representing 12% of the economically active population and 350000 families. (Min. Agricultura, 2019). However, jaggery consumption has sunk in the last decades because of change in consumer needs thus jeopardizing the entire jaggery agroindustry sector. In this regard, it is important to promote the use of jaggery in industrial foods, in particular in products of large consumption such as ice creams. Nevertheless, it is necessary to understand the impact of jaggery on the properties and characteristics of the final product. Then, it is important to understand the processes involved in ice cream manufacturing, the desired physicochemical and performance properties of the product, and the impact of the ingredients and the processes in such properties.

1.5 Ice cream manufacturing processes

As in many other processed food products, the manufacturing of ice cream involves a series of ingredients and steps to reach the desired set of characteristics that fulfills customer expectations. In this case, besides ingredients (see Table 1-1 and 1-2), the manufacturing process plays a major role in obtaining the desired characteristics of the commercial product (Chavez Montes, 2002). In general, the manufacturing process of ice cream involves steps of pasteurization, homogenization, ripening, aeration-freezing, hardening and final storage (Goff, Hartel, 2003).

Pasteurization: This step comes right after mixing the ingredients and enables the elimination of pathogens or bacteria that may damage the product. Most of the time it is made by subjecting the mixture at 82-87°C for 30 seconds. However, this might change depending on the pasteurization type (VAT – Slow; HTST - High Temperature/Short Time; UHT - Ultra-High Temperature)

Homogenization: Once pasteurized, the mixture is pumped through a very small orifice under a very high pressure drop between the entrance and the exit ports (i.e. from 8 to 18 MPa). This process breaks the fat into very small bubbles that are dispersed into the aqueous phase generating a more stable mixture. In general, the obtained fat globules have a maximum diameter of around 1µm.

Ripening: After cooling at 4°C, the product is maintained at this temperature for at least two hours and often overnight. The fat globules partially crystalize and the viscosity increases providing a structural development to the product.

Aeration and freezing: Once ripened, the solid mixture is processed in a scraped surface heat exchanger. Besides air incorporation, herein about 50% of the water is frozen and the fats are destabilized, enabling to stabilize the air bubbles.

Hardening: After aeration, the product is put on a plate freezer or within chambers or tunnels under a cold air flow (-45°C to -25°C) at 5 to 10 m.s-1. In this step around 80% of the water freezes and the product cools until it reaches -15°C at its core.

Storing: Above -25°C, ice crystals can grow and damage the product. Then the product can only be stored at -18°C for short periods, but for longer ones it has to be stored at -30°C.

1.6 Performance properties of ice cream and estimation from ingredients

In general, there is a large number of physicochemical properties that dictate the performance of an ice cream (Chavez Montes, 2002). However, for a rapid quality assessment and manufacturing control, a reduced number of them are suitable to screen among formulations, and to establish those with adequate behavior and promising performance. In this regard, the typical properties that need to be assessed during ice cream manufacturing, and consequently during ice cream design are: freezing point, overrun, density and viscosity.

1.6.1 Freezing point

Being a frozen dessert, it is essential to control the ice cream's freezing point. As the larger mass fraction corresponds to water, this property is mainly dictated by the concentration of solutes, namely sugars (including lactose) and mineral salts (Boutonnier, 2018). Usually, the mineral salts are mainly coming from the dairy ingredients, however, they are also present in non-negligible quantities in jaggery (ICONTEC, 2009). Then, a suitable combination of ingredients would enable to reach the required freezing point depression, which is the difference between the freezing point of pure water (0°C) and the temperature at which the mix starts to freeze. Interestingly, different authors have developed models based upon the ingredients to estimate the freezing points of sugar solutions. As already mentioned, these methods mainly consider the contribution of sugars and minerals content. The following equations can be used for the estimation of the freezing point of an ice cream mixture (Boutonnier, 2018):

- Step 1 : Calculation of the sugars' equivalence in sucrose with Equation (1.1).

$$SE = MSNF * L_{MSNF} + WS * L_{WS} + \sum_i A, i * FPD_i \quad (1.1)$$

Where,

SE: Equivalence of sucrose (%)

MSNF: Percentage of milk-solids-not-fat (MSNF) in the mix (%)

L_{MSNF}: Percentage of lactose in MSNF in the mix (%)

WS: Percentage of whey solids in the mix (%)

L_{WS}: Percentage of lactose in the whey solids in the mix (%)

A_i: Percentage of the sugar i in the mix in the mix (%)

FDP_i: Freezing point depression of the sugar i (ratio of the sugar i's molar mass and the sucrose's molar mass) in the mix

- Step 2 : Calculation of the concentration of the sugar's concentration in sucrose equivalence with Equation (1.2).

$$C_s = 100 \frac{SE}{100-TS} \quad (1.2)$$

Where,

C_s: Concentration of the sugar's concentration in sucrose equivalence (%)

TS: Percentage of total solids in the mix (%)

Step 3 : Reading of the freezing point depression associated with sugar in Table 1-6

Table 1-6: Freezing point depression of sucrose solutions

g Sucrose/ 100 g water	**FDP (°C)**	**g Sucrose/ 100 g water**	**FDP (°C)**	**g Sucrose/ 100 g water**	**FDP (°C)**
3	0.18	63	4.10	123	9.19
6	0.35	66	4.33	126	9.45
9	0.53	69	4.54	129	9.71
12	0.72	72	4.77	132	9.96
15	0.90	75	5.00	135	10.22
18	1.10	78	5.26	138	10.47
21	1.29	81	5.53	141	10.72
24	1.47	84	5.77	144	10.97
27	1.67	87	5.99	147	11.19
30	1.86	90	6.23	150	11.41
33	2.03	93	6.50	153	11.63
36	2.21	96	6.80	156	11.88
39	2.40	99	7.04	159	12.14
42	2.60	102	7.32	162	12.40
45	2.78	105	7.56	165	12.67
48	2.99	108	7.80	168	12.88
51	3.20	111	8.04	171	13.08
54	3.42	114	8.33	174	13.28
57	3.63	117	8.62	177	13.48
60	3.85	120	8.92	180	13.68

Source: (Boutonnier, 2018)

- Step 4 : Calculation of the freezing point depression associated with mineral salts with Equation (1.3).

$$FPD_s = \frac{S_{MSNF} * MSNF + S_{WS} * WS + S_{jaggery} * A_{jaggery}}{100 - TS} \quad (1.3)$$

Where,

FDP_S: Freezing point depression associated with the mineral salts (°C)

S_{MSNF}: Percentage of mineral salts in MSNF (%)

S_{WS}: Percentage of mineral salts in the whey solids (%)

$S_{jaggery}$: Percentage of mineral salts in jaggery (%)

$A_{jaggery}$: Percentage of the jaggery in the mix (%)

- Step 5 : The final freezing point depression is the sum of the freezing point depression associated with sugar and the freezing point depression associated with the mineral salts

1.6.2 Overrun

This is the ratio between the mass of the ice cream and the mass of the mix in the final product, and it is an indirect measurement of air content. It has an important impact on the product's viscosity such that, the higher the air content, the higher its viscosity. It is calculated with Equation (1.4).

$$OR = 100 \frac{m_m - m_{ic}}{m_{ic}} \tag{1.4}$$

Where,

OR: Overrun ratio (%)

m_{ic}: mass of a fixed volume of the ice cream (g)

m_m: mass at the same volume of the mix (g)

1.6.3 Density

It is an important trait of the product since it is one of the characteristics that allow the consumer to evaluate the category of the ice cream. Indeed, a heavy ice cream will be associated with a high standing ice cream whereas a light one will be associated with an economic one (Goff, Hartel, 2003). In the characterization of ice creams, two densities are calculated, namely the mix's one and the ice cream's one. They are calculated with Equations (1.5) and (1.6) respectively.

$$\rho_m = \frac{100}{\frac{F}{\rho_F} + \frac{TS-F}{\rho_{MSNF}} + 100 - TS} \quad (1.5)$$

$$\rho_{ic} = \frac{\rho_m}{\frac{OR}{100} + 1} \quad (1.6)$$

Where,

ρ_m: Density of the mix ($g \cdot L^{-1}$)

F: Percentage of fats (%)

ρ_F: Density of fats ($g \cdot L^{-1}$)

ρ_{MSNF}: Density of MSNF ($g \cdot L^{-1}$)

ρ_{ic}: Density of the ice cream ($g \cdot L^{-1}$)

1.6.4 Viscosity

The viscosity is one of the most important attributes of the product; the ice cream must not be too fluid or too hard. Similar to the density, the viscosity of both, the mix and the final product, can be calculated based upon the main ingredients. The mix is a non-Newtonian shear-thinning fluid. Its viscosity follows the Sisko model (Equation (1.7), (Chavez Montes, 2002)).

$$\eta_m = \eta_\infty + \kappa \dot{\gamma}^{n-1} \quad (1.7)$$

η_∞, κ, and n are parameters that depend mostly on the stabilizers' type and quantity, and are experimentally evaluated. The higher the number of stabilizers, the higher the ice cream's viscosity. The viscosity of the ice cream can be calculated with Equation (1.8)

$$\eta_{ic} = \eta_m \left(1 + \frac{1 + \frac{5\lambda}{2}}{1 + \lambda} \phi\right) \quad (1.8)$$

Where,

η_{ic}: Viscosity of the ice cream (Pa·s)

ϕ: Volume fraction of the air

λ: Ratio between the viscosity of the air and the viscosity of the mix (which can be neglected for ϕ<0,45)

2. Computer-aided design of ice creams containing jaggery

Product design is a complex task that is generally performed by expert personnel. Based upon a vast previous knowledge, design scientists develop prototype products that are later tested at different scales before being implemented at the industrial level. This process is highly resources-intensive, very ineffective and time-consuming, therefore accelerated methodologies for product design are hardly required. In this regard, computer-aided methodologies are suitable tools to boost product design and engineering. These methodologies involve the transformation of consumer and manufacturer needs, product performance properties, and processing operations into suitable interacting mathematical models that can be programmed to identify the optimal potential product. The mathematical optimization is done with respect to specific goals such as the expected product performance, manufacturing costs, energy consumption or even sustainability indicators, among others. Nevertheless, as the mathematical modeling involves simplifications, assumptions and it does not fully describe the complex and synergic phenomena (i.e. mixing, heat transfer, mass transfer and reaction), experimental validation of identified prototypes is still required. In this regard, integrated design methodologies are suitable to accelerate product development.

In general, computer-aided product design methodologies involve the assessment of consumer needs, their transformation into quantitative indicators to identify quality goals in terms of product performance, their correlation with physicochemical properties to enable an indirect assessment of needs fulfilment, and the prediction of such physicochemical properties from the ingredients and the processing conditions. This methodology can be then improved by integrating additional inputs such as manufacturing restrictions or policies (e.g. available ingredients or equipment, banned use of certain compounds) and systematized expert knowledge (i.e. heuristics). Such inputs and heuristics can be then transformed into inequalities or restrictions of the mathematical model, that can help to reduce the variables searching space for optimal solutions. By systematizing heuristics, it can be possible to narrow the number of ingredients and the range of concentration in the final products, to define suitable manufacturing policies, and to identify the range of operating conditions, among other advantages (Arrieta, 2020). Nonetheless, as in the heuristic process synthesis approach, the main disadvantage of heuristic-assisted product design is that it does not allow to obtain the global optimal solution. For instance, in food design products, heuristics are guiding the mixing policies during emulsification (e.g. order of addition of ingredients, mixer types and mixing rates, operating temperatures, etc.), but those might affect the organoleptic profile of the final product (Goff, Hartel, 2003). Besides, synergic effects are not completely understood, so heuristics related to the use of some ingredients might affect other properties in an unexpected way.

Then, despite the use of heuristics helping achieve a specific quality factor or process performance, the combination of all heuristics will divert from an overall optimal solution regarding the final design. Consequently, integration of experimental validation and consumer assessment is required to improve the product design methodology (Arrieta, 2018). In this case, a set of potential optimal solutions resulting from the model are prototyped at the lab scale, characterized and further assessed with experts or consumers. The outcomes from the assessment can then be used as guiding factors to modify the product design computer model, for instance by imposing weighting factors on the different performance properties, by adjusting ranges of acceptance regarding quality factors, or by imposing additional restrictions. This integrated methodology has been successfully applied in the design of structure products used in the cosmetics industry (Arrieta, 2018).

Considering all the above mentioned, the exploration of a computer-aided design methodology for ice creams including jaggery as a sweetener was divided into four stages. Initially a comprehensive literature review and consultation with experts were carried out to identify main formulation heuristics and constrains (e.g. technical, legal) to be fulfilled in the manufacture of ice creams. This stage also enabled the identification of main performance properties, and the determination of suitable models to assess the impact of the different ingredients, including jaggery, on the product properties. In a second stage, preliminary tests were carried out to assess how the jaggery could impact ice cream properties (e.g. density, viscosity, pH, texture, freezing point and melting rate). Thirdly, heuristics, restrictions, and mixture properties were transformed into mathematical equations suitable for a computer-aided ice cream design. In the last stage, optimization of the formulations was carried out based upon the computer model by minimizing the cost of the formulations. This was followed by experimental sensorial validation of the computer-generated designs which were prepared at the bench scale and finally assessed with panelists.

2.1 Conceptual framework for product design

The computer-aided method here used for ice cream design initially involved the identification of the main quality attributes of the product. For instance, consumers are able to identify the adequate body, texture, and melting properties of the product which are associated with the creaminess, softness, and certain structural semi-solid consistency. In turn, these attributes can be related through quality functions with physicochemical properties of the mixture such as melting rate and temperature, viscosity, density, etc. At the same time, these properties can be determined by functions that depend on the corresponding ingredients and the processing stages. At last, the processes are affected by a set of operating conditions and variables (e.g. mixing temperature, ingredients addition policy, stirring rates, etc.) (Bernardo & Saraiva, 2014). In this work, only the ingredients were changed during product design. The corresponding processing stages and operating conditions during ice cream manufacturing were fixed and defined according to literature review (Goff & Hartel, 2013) and from consultation with experts. These stages involved pasteurization, homogenization, ripening, aeration and freezing, hardening, and final storage.

2.2 Heuristics in ice cream design

Besides processing conditions, that in this case were maintained constant according to recommendations from literature and experts, the specific list of ingredients and the corresponding composition determines the physicochemical properties to the final product (e.g. density, viscosity, freezing point, etc.) as well as the sensory characteristics (e.g. color, taste, texture, etc.). As previously stated, the composition of an ice cream depends on the local regulations and the product's category (i.e. economy, standard, premium, superpremium), and some typical ranges of the composition of the different ingredients used in the formulation of ice creams were presented in Tables 1-1 and 1-2. These ranges are defined to ensure the expected performance of the product and to avoid undesired characteristics or bad quality. The corresponding functions and nature of the different ingredients typically used in ice cream formulations were presented in Tables 1-3 and 1-4. This information can be used to set the corresponding ranges of concentration for the formulation of ice creams. Then, the ranges of concentration of the different ingredients are summarized in Table 2-1.

Table 2-1: Suggested proportion of ingredients for hard-frozen ice cream products (Goff & Hartel, 2013)

Ingredient	Composition (% wt.)
Milk fat	10.0-16.0
Milk solids-non-fat	9.5-11.0
Sucrose	10.0-16.0
Corn syrup solids	0.0-5.0
Stabilizer*	0.15-0.35
Emulsifier*	0.0-0.15
Total solids	36.5- 41.65

* Highly variable depending on type; manufacturers recommendations are usually followed

Economical ice creams usually contain up to 36% of solids, including up to 10% of fats. When a blend of oils is used, it is advised to make sure that 30% to 70% of the fat is liquid between 4°C and 5°C for optimal partial coalescence (Goff & Hartel, 2013). Even though there is no heuristic about the balance between the oils and milk fats, it is relevant to limit the proportion of milk fat to half of the total fats in order to guarantee economic formulations. On the other hand, the Colombian law requires a minimum content of various items for dairy ice creams with vegetal oil (see Table 2-2).

Table 2-2: Colombian regulatory requirements (Min. Salud, 1989)

Item	Minimum content (% wt.)
Total fats	8
Milk fats	2
Milk solids on fat	11
Total solids	30
Milk proteins	2.5

2.3 Performance properties

In general, ice cream performance is indirectly assessed by the means of different physicochemical and sensory properties. Again, such properties can be affected by processing conditions and ingredients, but in this case only the effect of ingredients is assessed. The main properties used to characterize ice creams are: density, overrun, melting rate, freezing point, viscosity and sensory attributes. In the case of the sensory properties, they highly differ from one ice cream the other. Indeed, one could try to obtain a highly sweetened product whereas someone else could prefer to make a product with a moderated sweet taste. Besides, the sweet taste also depends on other ingredients. For instance, a chocolate ice cream needs a sweetener with higher sweetening powers than a vanilla ice cream in order to cover the cocoa's bitterness (Goff & Hartel, 2013). Thus, general rules in the incorporation of sugars and other ingredients with respect to sensory properties are not well established. Other attributes such as smoothness, mouthfeel and appearance are directly linked to the overrun ratio, the freezing point, the viscosity and the choice of the ingredients.

2.4 Translation of heuristics into equations and restrictions

2.4.1 Ingredients' heuristics

At this stage, the main performance properties of the ice cream are predicted from ingredients by using suitable mixing rules based upon the collected heuristics, the corresponding mass balances, and equations reported in section 1.6. Additionally, the total solid content (TS) is calculated with Equation (2.1), the content of liquid oils (LO) at 4-5°C is calculated with Equation (2.2) and the dairy fats content (MF) is calculated with Equation (2.3). The total content of fats (F), milk proteins (P) and the milk solids-non-fat ($MSNF$) are calculated with Equation (2.4), (2.5), and (2.6), respectively.

$$TS = \sum_i (A_i + F + MSNF + E, S) \tag{2.1}$$

$$LO = \sum_i O, i \times LO, i \tag{2.2}$$

$$MF = \sum_i (D, i \times MF, D, i) \tag{2.3}$$

$$F = MF + \sum_i O, i \tag{2.4}$$

$$P = \sum_i (D,i \times P,D,i) \tag{2.5}$$

$$MSNF = \sum_i (D,i \times MSNF,D,i) \tag{2.6}$$

Where,

E,S : Percentage of emulsifier-stabilizer (%)

O,i : Percentage of oil i in the mix (%)

LO,i : Proportion of liquid oil i at 4-5°C (%)

D,i : Percentage of dairy product i in the mix (%)

MF,D,i : Percentage of milk fats in dairy product i (%)

P,D,i : Percentage of milk proteins in dairy product i (%)

$MSNF,D,i$: Percentage of milk solids non fats in dairy product i (%)

2.4.2 Formulation constraints

Restrictions established by the Colombian regulatory agencies regarding ice cream physicochemical properties, and those defined by expert knowledge, were defined as the inequalities described in Equations (2.7) to (2.13) (Min. Salud, 1989).

$$30 \leq TS \leq 36 \tag{2.7}$$

$$30 \leq LO \leq 70 \tag{2.8}$$

$$MF \geq 2 \tag{2.9}$$

$$MF \leq F/2 \tag{2.10}$$

$$F \geq 8 \tag{2.11}$$

$$P \geq 2.5 \tag{2.12}$$

$$MSNF \geq 11 \tag{2.13}$$

The required water content (W_{req}) and the actual water loading (W_{actual}) were calculated with Equations (2.14) and (2.15), respectively.

$$W_{req} = 100 - TS \tag{2.14}$$

$$W_{actual} = \sum_i (100 - MSNF, D, i - MF, D, i) \times D, i \tag{2.15}$$

Only if in a guessed formulation the actual water loading is lower than the required, the computer program returns a formulation in which water is added as an ingredient.

The density of the mixture is a property that can be fixed arbitrarily because it highly depends on the air content, but must be higher than 475 g/L according to Colombian regulations (Min. Salud 1989). Once density is fixed, the computer model returns the required overrun of the product by using the inverse of the density of the mix ($invd_m$) which is calculated with Equation (2.16) (Boutonnier, 2018).

$$invd_m = \frac{MF}{\rho_{MF}} + \frac{W}{\rho_W} + \frac{TS-F}{\rho_{DE}} + \sum_i \frac{O,i}{\rho_{O,i}} \tag{2.16}$$

The density of milk fats (ρ_{MF}) is estimated at 0.93 kg/L (Boutonnier, 2018). Then, using the inverse of the density of the mix and sought ice cream's density, the required overrun (OR_{req}) can be estimated with Equation (2.17).

$$OR_{req} = 100 * \left(\frac{1}{d * invd_m} - 1\right) \tag{2.17}$$

The corresponding cost of a given formulation can be calculated with Equation (2.18), using the costs of the ingredients (to be set by the user of the computer program) and their loadings in the final mix. The specific costs for the ingredients used in the experimental validation at bench scale are reported in Table 2-3.

$$cost = m_{tot} * \sum_i cost_{ing,i} \times Ing_i \tag{2.18}$$

In order to assess the potential sensory impacts of using jaggery as a sweetener, it was decided to prepare a vanilla ice cream. Besides being the largest consumed in the country, the plain flavor of vanilla ice cream avoids masking potential sensory effects of jaggery. According to expert knowledge, to obtain a tasty vanilla ice cream, one milliliter of vanilla essence per kg of mix must be added to the formulation.

Table 2-3: Unitary costs of ice cream ingredients

Category	Ingredient	Cost (USD/kg)
Dairy products	Liquid milk	0.96
	Milk powder	3.02
	Dairy cream	3.75
Nondairy fat	Palm oil	0,69
Sweetener	Refined sugar	0.35
	Jaggery	1.09
Emulsifier- Stabilizer	Cremodan	90.00
Flavoring	Vanilla essence	48.97

2.4.3 Computer modeling and optimization

The previous set of equations was programed in Python®. The use of the Pyomo® library enables to create a model, including constraints, and to set the objective function which is the total cost of ingredients here. The problem being linear, the GLPK solver is adequate for optimization (Hart et al., 2012). The corresponding optimization problem was the minimization of total ingredients costs (Equation 2.18). The problem resulted in a deterministic global optimization generating a single solution: the exact quantity of the ingredients to be put in the formulation guaranteeing compliance with heuristics, regulations and user's requirements with the lowest cost. In order to permit product designer participation and to enable using most updated costs, the program was set in such a way that the user has to select the ingredients among those available in Table 2-4 and indicate their characteristics (fat and milk-solids-non-fat percentage for dairy products, percentage of jaggery among the sweeteners, price), required density, sweetening power and mass of the batch. For simplification matters, the emulsifier-stabilizer and flavor are specified by the program.

Table 2-4: Available ingredients in the computer program

Type of ingredient	Ingredient
Dairy products	Liquid milk
	Milk powder
	Dairy cream
Sweeteners	Sugarcane
	Jaggery
Fats	Palm oil
	Palm kernel oil
	Butterfat,
	Coconut oil
	Sunflower oil
	Peanut oil

2.5 Prototype ice cream formulation, manufacture and characterization

The above-mentioned heuristics and restrictions have been identified for traditional ice cream formulations sweetened with refined sugar or glucose syrup. However, jaggery addition might generate changes in the properties and performance of typical ice cream formulations. Then, in order to assess the impact of jaggery, a blank sample only containing sugar as a sweetener (M1 and duplicate M2) and another with only jaggery (M3 and duplicate M4) were prepared with the formulations shown in Table 2-5. This mixture corresponds to a base case that was defined considering regulations and heuristics.

Table 2-5: Composition of ice cream mixes for preliminary tests

Ingredients	Concentration (% wt.)	
	M1/M2	M3/M4
Water	62.8	62.3
Skim milk powder	11.4	11.4
Dairy cream	5.5	5.5
Palm oil	6.0	6.0
Sugar cane	13.9	0
Jaggery	0	14.4
Cremodan®	0.4	0.4

The manufacturing process is a simplified version of the steps briefly described in the first chapter. After ingredient weighing, the mixtures were homogenized for 5 minutes at 12 000 rpm with an Ultra-Turrax®, pasteurized at approximatively 77°C for 10 minutes in a bain-marie, and aged overnight at 4°C. The mixtures were then whipped for five minutes and poured into an ice cream maker (Whynter ICM-200LS®) where they were frozen and aerated for 30 minutes. Once obtained, the mixes were characterized by measuring density, pH, freezing point and viscosity and ice creams were characterized by measuring texture, overrun and melting rate.

Density was measured using a 10 ml calibrated pycnometer with a 4 x 10^{-4} ml uncertainty. Overrun of the samples was measured by comparing the weight of a pycnometer filled with mix and the same pycnometer filled with ice cream after batch freezing. Viscosity was measured with a viscosimeter (VT550®) for each mix at room temperature. pH was measured for each mix with a pH-meter (F20 Mettler Toledo with a 0.01 precision) Texture was measured with a texture analyzer (TA.XTplus Texture Analyzer®) right after taking the samples from the freezer, and it was remeasured 3, 6 and 9 minutes later in order to observe the evolution of texture with time. The freezing point was measured by differential scanning calorimetry (DSC) using a Metler DSC1. A ~20 mg sample was placed within an aluminum crucible and it was subjected to cooling up to -60 °C and subsequent heating up to 25 °C, both at a 5 °C/min rate, and under a Nitrogen blanket. The reported melting temperature corresponded to the onset peak temperature during the heating part of the experiment. The melting rate of weighed samples of each ice cream was measured gravimetrically, letting a sample of 20 g of ice cream to melt and drip over a plate located on a balance, and following change of weight with time at room temperature.

2.6 Sensory assessment of optimal formulation

The optimal formulations of ice cream obtained from the computer model were prepared following the same procedure described in the previous section. Once obtained, the products were subjected to assessment with 55 ice cream consumers from a population of individuals of ages in-between 15 to 80 years, and different socioeconomic backgrounds. Participants were blind to the nature of the ingredients but they knew the product corresponded to ice cream. They were given the samples in an aleatory order and an assessment form to fill in. For each sample, five attributes were assessed using a simple assessment tool, namely a five-point hedonic scale. The assessed attributes were easily determined by the panelist, and they corresponded to: color, general flavor, sweet taste, vanilla flavor and texture. After each sample assessment, the panelists had to rinse their mouth with water to avoid biased evaluation of subsequent samples. Once the data was collected from the evaluation forms, it was uploaded to an electronic data base for further statistical analysis.

The statistical analysis was carried out via a principal component analysis using a MATLAB® macro. This was done in order to assess whether the general evaluation of a sample is significantly different from another sample with a 95% significance. The first step is to assess how many components (out of 5 for 5 attributes) are worth studying. They are considered to be worth studying if their eigenvalue is above 1, otherwise they constitute noise (Cliff, 1988). The second step is to do the PCA based on the number of components that are worth studying and with them, generate a score plot. If less than 2 components are worth studying, the score plot must still be made based on 2 components in order to obtain a graph. Finally, a Tukey-Kramer test was run in JMP® to observe the evaluation of each attribute individually and to see if jaggery concentrations would generate better or worse product performance.

3. Results and discussion

3.1 Ice cream modeling

The heuristics and constraints were successfully coded in Python®, and the resulting program is presented in Annex 1. In the end, the system had numerous variables and equations, including five independent equations and nine variables which means four parameters to vary to solve the system: dairy cream, liquid milk, milk powder and vegetal oil content. The computer program was solved on a Lenovo® 81N6 computer with 8GB RAM and always gave a single formulation in 0.07 seconds. For each ingredient, it returned the mass and mass percentage, and returned an error message if no solution is found.

3.2 Preliminary assessment of jaggery impacts on ice cream formulations

The properties of the base case samples sweetened with sugar (M1 and M2) or jaggery (M3 and M4), formulated as described in Table 2-1, are presented in this section. As observed in Table 3-1, density, overrun capacity and pH of the four samples did not present significant differences. This was an interesting result that indicates that jaggery does not change the properties of the mixture when replacing refined sugar. This was expected as the sweetener is only a part of the formulation (14 % wt.), and because jaggery is mainly constituted of sucrose. The deviations in the properties might be related to the impacts of reducing sugars and mineral material.

Table 3-1: Density and overrun capacity of ice cream mixes

Formulation	Density (~16°C)	Overrun capacity	pH (~17°C)
M1	1,095	39%	6,64
M2	1,128	41%	6,71
M3	1,120	42%	6,47
M4	1,088	43%	6,43

Once the properties were evaluated, only one sample of each ice cream containing either refined sugar or jaggery was subjected to melting behavior analysis; these corresponded to samples M1 and M3. As observed in Figure 3-1, the ice cream containing refined sugar (i.e. M1) starts to melt before the one containing jaggery (M3). This indicates that jaggery enhances the solid structure, reducing melting rates and air losses from the structure. This is interesting because jaggery loading could be even reduced further to obtain a similar behavior to that of samples sweetened with refined sugar. Nonetheless both curves presented a similar behavior once it starts melting, verifying that jaggery does not change the properties of the ice cream.

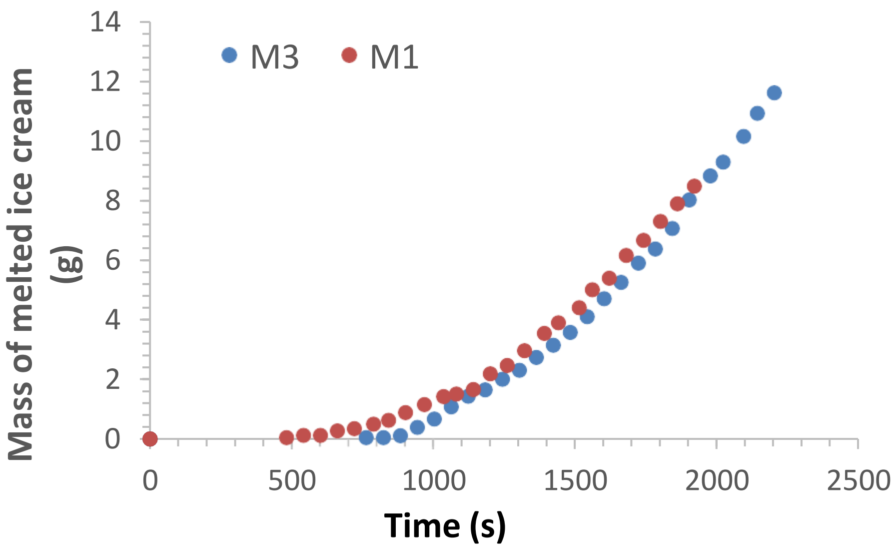
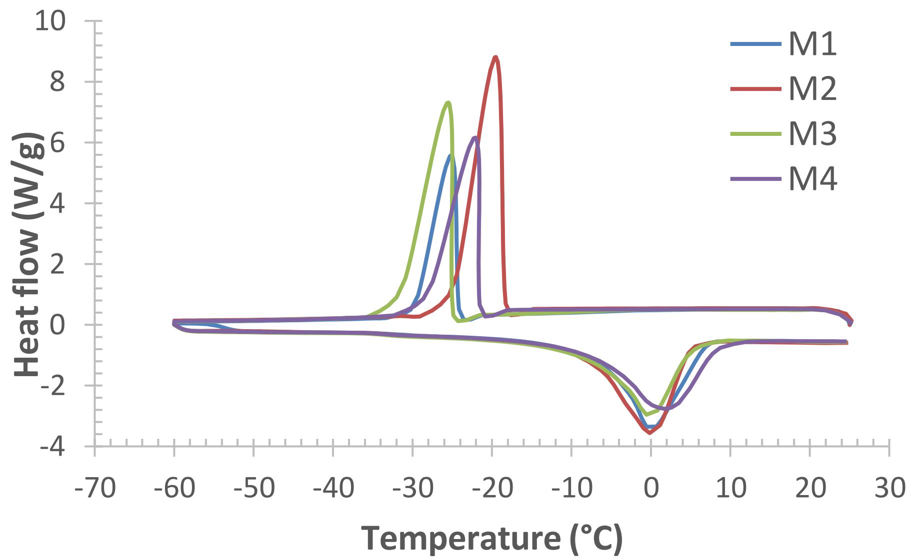


Figure 3-1: Melting rate of ice cream samples at ambient conditions. M1 sweetened with sugar and M3 sweetened with jaggery

The DSC profiles of the samples are presented in Figure 3-2 in a differential scanning calorimetry diagram. The positive peaks indicate complete solidification and crystallization of the mixes, whereas the negative peaks describe the melting process. The change in the size and position of the crystallization peaks is related to the slightly different weight of the samples because this process is kinetically driven (Höhne et al., 2003). In contrast deviations of peak locations in the melting process are minor because the process is spontaneous and readily done. Despite the small variations, the onset temperature of the melting peaks is similar in all samples either containing jaggery or refined sugar. Interestingly, the melting point of the ice cream mixture is around 0 ºC, being close to that of water. Moreover, the heat of fusion is 3.47 W/g on average for samples sweetened with refined sugar and 2.81 W/g on average for samples sweetened with jaggery which is quite comparable.

Figure 3-2: DSC profile of ice cream samples. M1 and M2 are sweetened with sugar. M3 and M4 sweetened with jaggery



The rheological behavior of the mixes was also studied, and the resulting profiles are presented in Figures 3-3 and 3-4. As observed, the average dynamic viscosity of the mixes containing jaggery is slightly higher than that prepared with refined sugar; still, both have similar dynamic viscosity at different shear stresses. The same conclusion can be made with the tangential stress in Figure 3-4. This is an important result that indicates that mixing conditions during ice cream aeration will not change much if manufactures decide to substitute refine sugar with jaggery.

Figure 3-3: Dynamic viscosity vs shear stress

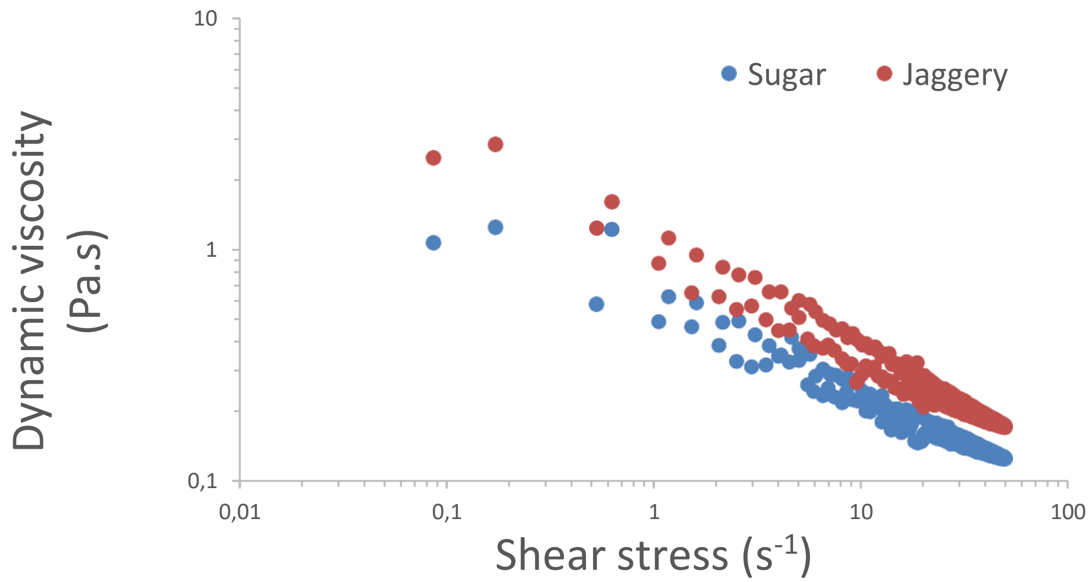
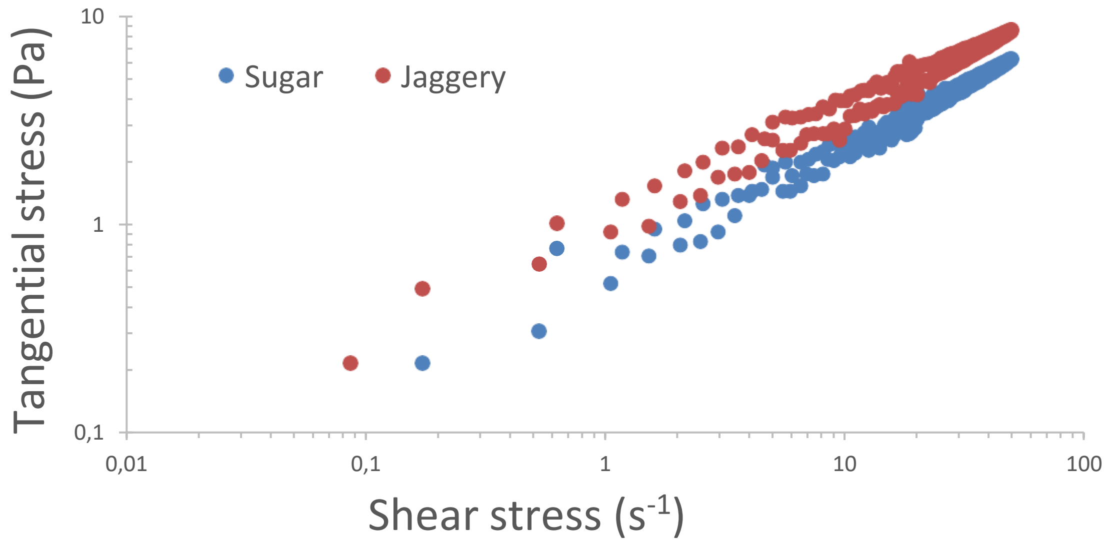
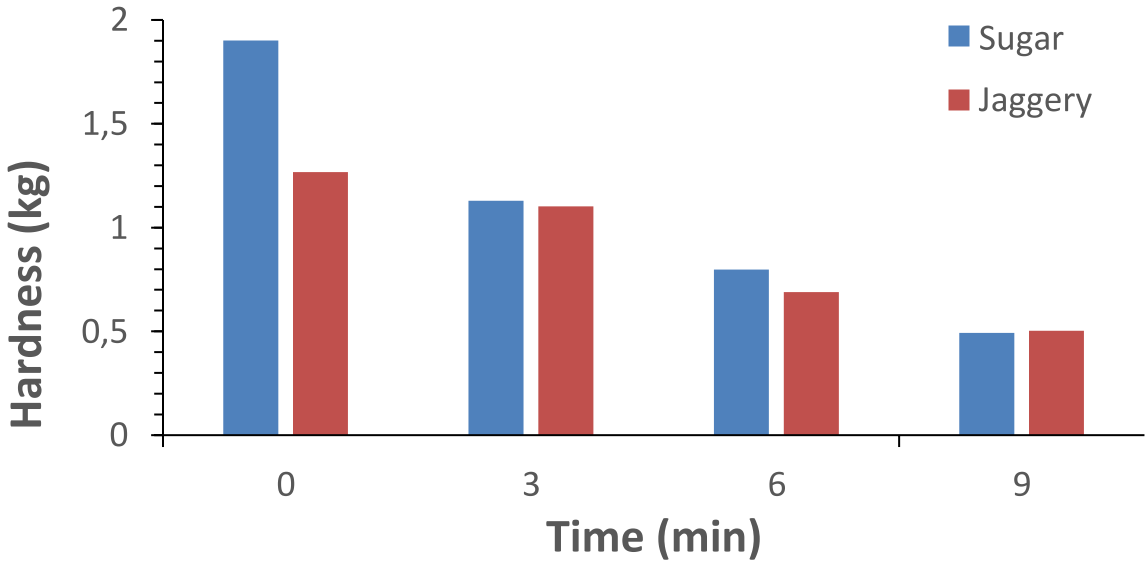


Figure 3-4: Tangential stress vs shear stress



The hardness of the ice cream was also evaluated for all samples, and it is presented in Figure 3-5. As expected, the average hardness of the ice cream is higher for the samples just removed from the freezer and it decreases over time. Interestingly, the sample sweetened with refined sugar exhibits a rapid decrease in hardness. This is consistent with the observed rapid melting of Figure 3-1. However, after a few minutes, both samples behave similarly, which coincides with the melting rate analysis.

Figure 3-5: Evolution of ice cream's hardness with time



A fundamental result of the preliminary experiments was that there was no need to include modifications to the equations used to predict the properties of the mixture when replacing refined sugar with jaggery. This was valuable as the available heuristic could be applied in the case of jaggery-added ice creams. Still, sensory properties need to be assessed, and those will be explored in a subsequent section.

3.3 Computer-aided design and sensory assessment

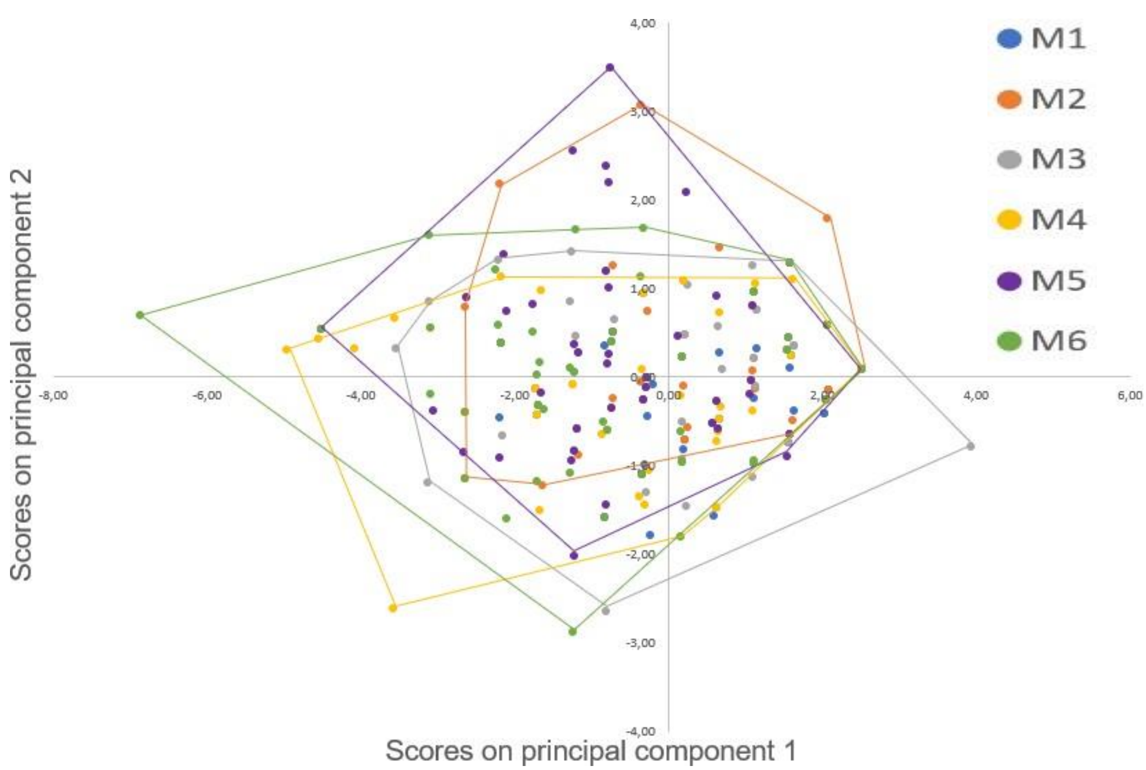
Palm oil, being economic and widely available in Colombia, was used to formulate the ice creams that were assessed in the sensorial analysis. After computer design, the program returned six formulations that are presented in Table 3-2, and they contained jaggery as a substitute for refined sugar. As observed, the sweetening level was maintained constant in all samples (jaggery's sweetening power being estimated at 0.97 and refined sugar's at 1), but jaggery substituted 0%, 20%, 40%, 60%, 80% and 100% of the total sweetener loading, respectively. The remaining amount of sweetener corresponded to refined sugar.

Table 3-2: Composition of ice cream mixes for sensorial analysis

Ingredients (%)	Formulations					
	M1	M2	M3	M4	M5	M6
Liquid milk	75,9	75,9	75,8	75,7	75,7	75,6
Skim milk powder	4,9	4,9	4,9	4,9	4,9	4,9
Palm oil	5,7	5,7	5,7	5,7	5,7	5,7
Sugar cane	13,1	10,5	7,9	5,3	2,7	0
Jaggery	0	2,6	5,3	8,0	10,7	13,4
Cremodan ®	0.4	0.4	0,4	0.4	0.4	0,4

After the panelists tested the different samples and the results were processed in the software, a PCA was made to see if they could differentiate the ice creams in terms of general sensorial perception. This involved assessment of color, general flavor, sweet taste, vanilla flavor and texture. As a result of the PCA, only one component had an eigenvalue higher than one, so the score plot was based on a 2-component basis (Figure 3-6).

Figure 3-6: PCA score plot of assessed samples.



As observed in Figure 3-6, all convex hulls are overlapped, indicating that the panelist did not find differences among samples. In general, all of them are perceived as similar products. Nevertheless, the use of the Tukey-Kramer analysis method (Table 3-3) showed that, apart from texture, the assessments of all studied attributes are significantly influenced by the jaggery content. Indeed, the formulations for each attributes apart from texture are not all connected by the same letter. For the evaluation of a given attribute, a formulation having one or several letters is not significantly different from any formulation that has at least one letter in common. For instance, according to Table 3-3, M3 is not significantly different than any other formulation in terms of color but M1 and M6 are significantly different.

Table 3-3: Tukey-Kramer test (formulations not connected by the same letter are significantly different).

Color

Formulation				Mean
M1	A			4.5636364
M2	A	B		4.2909091
M3	A	B	C	4.1454545
M4		B	C	4.0363636
M6		B	C	3.8545455
M5			C	3.8000000

General flavor

Formulation			Mean
M1	A		4.3454545
M2	A	B	4.0545455
M3	A	B	4.0000000
M6		B	3.8181818
M4		B	3.7818182
M5		B	3.7272727

Vanilla flavor

Formulation				Mean
M1	A			4.1272727
M2	A	B		4.0000000
M5	A	B	C	3.6545455
M3	A	B	C	3.6363636
M4		B	C	3.5454545
M6			C	3.2545455

Sweet taste

Formulation			Mean
M2	A		4.1818182
M1	A		4.1454545
M3	A	B	3.9090909
M5	A	B	3.7090909
M6		B	3.6363636
M4		B	3.5272727

Texture

Formulation		Mean
M1	A	4.2000000
M2	A	4.1090909
M4	A	3.9636364
M5	A	3.9454545
M6	A	3.9454545
M3	A	3.8545455

The formulations with lower contents of jaggery showed better acceptance of color. Indeed, jaggery gives a caramel-like color (which intensity increases with the jaggery content in the mix) to the ice cream. It is important to recall that consumers expect vanilla ice cream to be white. This explains that the highest rated sample in terms of color was the sample without jaggery. Nonetheless, it appears that the replacement of sugar by jaggery does not affect the acceptance of the color if less than 40% of the sugar is replaced. Moreover, jaggery contains volatile aromatic components (García et al., 2017) that can affect the general flavor of ice cream and partially covers the vanilla flavor. Therefore, samples with lower jaggery content showed a higher acceptance in terms of taste. The protein content of jaggery may also have an impact on its sweet taste, making it appear less sweet than white sugar. This would explain that again, samples with lower jaggery content show better acceptance for sweet taste. Up to 40% of refined sugar can be replaced by jaggery without impacting the acceptance of this attribute. Nonetheless, on this attribute, it appears that the sample with an 80% refined sugar substitution was still well accepted.

From the sensory analysis it can be concluded that in general, up to 40% of the refined sugar can be substituted with jaggery in a vanilla ice cream formulation without any adjustment being required. It is important to underline that even though differences in the average rating of each attribute are observed, they are relatively small. The largest value was 0.88 units between the average rating for the vanilla flavor of M1 and M6. Results also suggest that jaggery would be better suited for chocolate or caramel-like ice creams, as those have similar flavor and color profiles.

4. Conclusions and recommendations

4.1 Conclusions

This work developed a successful computer-aided design method suitable for ice creams formulation using an integrated heuristic approach. Heuristic and expert knowledge were transformed into mathematical models that enable the prediction of the main physicochemical and major performance properties of ice cream mixtures based upon their ingredients. Once obtained, the method was tested and validated in the formulation of ice creams containing jaggery as a substitute for refined sugar.

From the physicochemical characterization of the ice cream samples via density, melting point, melting rate, rheology, and hardness evaluation, it was found that jaggery does not significantly affect the characteristics of the ice cream with respect to those samples sweetened with only refined sugar. In addition to this, the overall sensorial perception of samples was similar among samples with different content of jaggery. The largest differences among attributes of samples with a variable content of jaggery were in color and taste. Particularly, this occurred in samples where jaggery represented more than 40% of the sweetener loading. As for the sweet taste differences, it can be concluded that the jaggery's sweetening power was overestimated in the program and should be adjusted in the code. This can be related to the masking effect of reducing sugars or minor components in jaggery (e.g. proteins, flavonoids).

4.2 Recommendations

To counteract the effects of jaggery, it could be interesting to develop darker ice creams with stronger flavors or flavors closer to jaggery's such as chocolate, caramel or *dulce de leche*, so that the influence of the color and taste of jaggery would be mitigated. Also, since jaggery has its own flavor a jaggery-flavored ice cream could be developed. These results encourage the development of jaggery-containing ice creams on an industrial scale and further, the inclusion of jagger in other food products. It would be interesting to further develop the program to include other sweeteners that are widely used in the frozen dessert industry.

Annex : Ice cream design code

The program returns the total cost of the formulation, the mass of each ingredient in kg and their proportion. The code was used to obtain the formulations reported in Table 3-2. It returned barely legal formulations, and all heuristics matched values near the legally accepted limits.

To use the program, the user has to input the ingredients to be used, among those described in Table 2-4 and indicate their price. They also have to indicate the cost per kg of each ingredient and milk solids non fat and milk fats content of each dairy product. The user is also able to fix the sweet level of the final product, the desired density (which must be higher than 475 g/L to respect Colombian regulations) and the mass of the batch.

Generally, jaggery is more expensive than refined sugar, therefore it was decided that the percentage of refined sugar replaced by jaggery must be fixed by the user in order to prevent the program from always giving formulations with no jaggery content. Moreover, dairy cream being more expensive than other dairy products, the program tends to minimize its use, favoring the use of milk powder and liquid milk to fulfill the MSNF and MF requirements. For economic reasons, palm oil is preferred rather than other vegetal oils. Moreover, this oil does not require to be mixed with vegetal oils since a suitable proportion of this oil is liquid at 4-5°C. The quantity of vanilla essence to be included in the ice cream was fixed at 1mL per kg of mix according to experts' input. The quantity of Cremodan SE46-2 (emulsifier-stabilizer) to be included was fixed at 0.40% wt. based on its technical specification for an ice cream containing an 8% fat content (the legal minimum).

Python Code

```
from pyomo.environ import *
import pyomo.environ as pyo
from pyomo.opt import SolverFactory

#PARAMETERS: #Inician con e0

#Non-modifiable parameters
```

```
#1.    Sweetening power of white sugar cane
e0_sp1=0.99
#2.    Sweetening power of jaggery
e0_sp2=0.97
#3.    Water density (g/L)
e0_rho_w=1000
#4.    Cremodan mass fraction in the mix
e0_w_em1=0.004
#5.    Density of palm kernel oil
e0_pko_d=0.92
#6.    Density of butterfat
e0_bf_d = 0.93
#7.    Density of coconut oil
e0_co_d = 0.96
#8.    Density of sunflower oil: 0.918 - 0.923
e0_so_d = 0.921
#9.    Density of palm oil
e0_palmo_d = 0.92
#10.    Density of peanut oil: 0.912 - 0.920
e0_peano_d = 0.916

# Decalaration du modele
#model = pyo.ConcreteModel()
model = pyo.ConcreteModel()


#model mass
model.mass_Liquid_milk = pyo.Var(domain=NonNegativeReals)
model.mass_Powdered_milk = pyo.Var(domain=NonNegativeReals)
model.mass_Dairy_cream = pyo.Var(domain=NonNegativeReals)
model.mass_White_sugarcane = pyo.Var(domain=NonNegativeReals)
model.mass_Jaggery = pyo.Var(domain=NonNegativeReals)
model.mass_Palm_oil = pyo.Var(domain=NonNegativeReals)
model.mass_Sunflower_oil = pyo.Var(domain=NonNegativeReals)
model.mass_Coconut_oil = pyo.Var(domain=NonNegativeReals)
model.mass_Palm_kernel_oil = pyo.Var(domain=NonNegativeReals)
model.mass_Peanut_oil = pyo.Var(domain=NonNegativeReals)
model.mass_Butterfat = pyo.Var(domain=NonNegativeReals)
model.mass_Cremodan= pyo.Var(domain=NonNegativeReals)
model.mass_Vanilla_essence= pyo.Var(domain=NonNegativeReals)
model.mass_Water= pyo.Var(domain=NonNegativeReals)


#Modifiable parameters given by the user
#Prices are initially set at 0

e0_c_wsc=0
e0_c_j =0
e0_c_po=0
e0_c_so=0
```

```
e0_c_co=0
e0_c_pko=0
e0_c_peo=0
e0_c_lm = 0
e0_c_pm=0
e0_c_dc=0
e0_c_b=0
e0_c_w=0

uselm="no"
usedc="no"
usepm="no"
while (uselm=="no" or uselm=="No") and (usepm=="no" or usepm=="No") and
(usedc=="no" or usedc=="No"):
    e0_wf_lm=0
    e0_wmsnf_lm=0
    e0_wp_lm=0
    print('At least one dairy product must be used')
    print ('Will liquid milk be used ? (Yes or no) ')
    cpt=0
    while cpt==0:
        uselm=str(input())
        if uselm=="Yes" or uselm=="yes":
            model.mass_Liquid_milk_constraint_1 = pyo.Constraint(expr =
model.mass_Liquid_milk>=.01)
            print('Enter the mass fraction of fat in liquid milk')
            e0_wf_lm = float(input())
            while e0_wf_lm>1 or e0_wf_lm<0:
                print("Mass fraction of fat in liquid milk must be
between 0 and 1")
                print('Enter the mass fraction of fat in liquid milk')
                e0_wf_lm = float(input())
            print('Enter the mass fraction of proteins in liquid milk')
            e0_wp_lm = float(input())
            while e0_wp_lm>1 or e0_wp_lm<0:
                print("Mass fraction of proteins in liquid milk must be
between 0 and 1")
                print('Enter the mass fraction of proteins in liquid
milk')
                e0_wp_lm = float(input())
            print('Enter the mass fraction of milk-solids-non-fat in
liquid milk')
            e0_wmsnf_lm = float(input())
            while e0_wmsnf_lm>1 or e0_wmsnf_lm<0:
                print("Mass fraction of milk-solids-non-fat in liquid
milk must be between 0 and 1")
                print('Enter the mass fraction of milk-solids-non-fat in
liquid milk')
                e0_wmsnf_lm = float(input())
            print('Enter the cost of liquid milk per kg')
            e0_c_lsm = float(input())
            while e0_c_lsm<0:
                print('Price cannot be a negative value')
```

```
                print('Enter the cost of liquid milk per kg')
                e0_c_lsm = float(input())
            cpt=1
        elif uselm=="No" or uselm=="no":
            model.mass_Liquid_milk_constraint_1 = pyo.Constraint(expr =
model.mass_Liquid_milk ==0)
            cpt=1
        else:
            print('The answer must be yes or no')
    e0_wf_dc=0
    e0_wmsnf_dc=0
    e0_wp_dc=0
    print ('Will dairy cream be used ? (Yes or no) ')
    cpt=0
    while cpt==0:
        usedc=str(input())
        if usedc=="Yes" or usedc=="yes":
            model.mass_Dairy_cream_constraint_1 = pyo.Constraint(expr =
model.mass_Dairy_cream >=.01)
            print('Enter the mass fraction of fat in dairy cream')
            e0_wf_dc = float(input())
            while e0_wf_dc>1 or e0_wf_dc<0:
                print("Mass fraction of fat in dairy cream must be
between 0 and 1")
                print('Enter the mass fraction of fat in dairy cream')
                e0_wf_dc = float(input())
            cpt=1
            print('Enter the mass fraction of proteins in dairy cream')
            e0_wp_dc = float(input())
            while e0_wp_dc>1 or e0_wp_dc<0:
                print("Mass fraction of proteins in dairy cream must be
between 0 and 1")
                print('Enter the mass fraction of proteins in dairy
cream')
                e0_wp_dc = float(input())
            print('Enter the mass fraction of milk-solids-not-fat in
dairy cream')
            e0_wmsnf_dc = float(input())
            while e0_wmsnf_dc>1 or e0_wmsnf_dc<0:
                print("Mass fraction of fat in milk-solids-not-fat in
dairy cream must be between 0 and 1")
                print('Enter the mass fraction of milk-solids-not-fat in
dairy cream')
                e0_wmsnf_dc = float(input())
            print('Enter the cost of dairy cream per kg')
            e0_c_dc = float(input())
            while e0_c_dc<0:
                print('Price cannot be a negative value')
                print('Enter the cost of dairy cream per kg')
                e0_c_dc = float(input())
```

```
        elif usedc=="No" or usedc=="no":
            model.mass_Dairy_cream_constraint_1 = pyo.Constraint(expr =
model.mass_Dairy_cream ==0)
            cpt=1
        else:
            print('The answer must be yes or no')

    e0_wf_pm=0
    e0_wmsnf_pm=0
    e0_wp_pm=0
    print ('Will powdered milk be used ? (Yes or no) ')
    cpt=0
    while cpt==0:
        usepm=str(input())
        if usepm=="Yes" or usepm=="yes":
            model.mass_Powdered_milk_constraint_1 = pyo.Constraint(expr
=  model.mass_Powdered_milk >=.01)
            print('Enter the mass fraction of fat in powdered milk')
            e0_wf_pm = float(input())
            while e0_wf_pm>1 or e0_wf_pm<0:
                print("Mass fraction of fat in powdered milk must be
between 0 and 1")
                print('Enter the mass fraction of fat in powdered milk')
                e0_wf_pm = float(input())
            cpt=1
            print('Enter the mass fraction of proteins in powdered
milk')
            e0_wp_pm = float(input())
            while e0_wp_pm>1 or e0_wp_pm<0:
                print("Mass fraction of proteins in powdered milk must
be between 0 and 1")
                print('Enter the mass fraction of proteins in powdered
milk')
                e0_wp_pm = float(input())
            print('Enter the mass fraction of milk-solids-non-fat in
powdered milk')
            e0_wmsnf_pm = float(input())
            while e0_wmsnf_pm>1 or e0_wmsnf_pm<0:
                print("Mass fraction of milk-solids-non-fat in powdered
milk cannot be greater than 1")
                print('Enter the mass fraction of milk-solids-non-fat in
powdered milk')
                e0_wmsnf_pm = float(input())
            print('Enter the cost of powdered milk per kg')
            e0_c_p = float(input())
            while e0_c_p<0:
                print('Price cannot be a negative value')
                print('Enter the cost of powdered milk per kg')
                e0_c_p = float(input())
        elif usepm=="No" or usepm=="no":
            model.mass_Powdered_milk_constraint_1 = pyo.Constraint(expr
=  model.mass_Powdered_milk ==0)
            cpt=1
```

```
        else:
            print('The answer must be yes or no')

print('Enter the desired density of the ice cream in g/L')
e0_packw = float(input())
while e0_packw<475:
    print('According to the Colombian law, the density of the ice cream
must be more than 475 g/L')
    print('Enter the desired density of the ice cream in g/L')
    e0_packw = float(input())
print('Enter the total mass of the mix batch in kg')
e0_totalm = float(input())
while e0_totalm<=0:
    print('The total mass of the batch must be strictly positive')
    print('Enter the mass of the mix batch in kg')
    e0_totalm = float(input())
print('Enter the sweetnening power target value; A value between 0.12-
0.14 is recommended')
e0_sp_t = float(input())
while e0_sp_t<=0 or e0_sp_t>1:
    print('The sweetning power target value must be strictly positive
and lower than 1')
    print('Enter the sweetnening power target value; A value between
0.12-0.14 is recommended')
    e0_sp_t = float(input())

#Sweeteners
print("In that list, how many sweeteners must be included ? (Sugar,
jaggery)")
nbsweeteners=int(input())
while nbsweeteners>2 or nbsweeteners==0 :
    print("Sweeteners are mandatory and up to two sweeteners can be
used")
    print("In that list, how many sweeteners must be included ? (Sugar,
jaggery)")
    nbsweeteners=int(input())
sweet=[0]*nbsweeteners
cpt=0
if nbsweeteners<2:
    print("What sweetener must be included, sugar or jaggery ?")
    while cpt<nbsweeteners:
        sweet[cpt]=str(input())
        if sweet[cpt]=="sugar" or sweet[cpt]=="Sugar":
            cpt=cpt+1
        elif sweet[cpt]=="jaggery" or sweet[cpt]=="Jaggery":
            cpt=cpt+1
        else:
            cpt=0
            print("Please select only sugar or jaggery")
```

```
if len(sweet)==1:
    if sweet[0]=="sugar" or sweet[0]=="Sugar":
        print('Enter the cost of white sugar cane per kg')
        e0_c_wsc = float(input())
        while e0_c_wsc<0:
            print('Cost cannot be a negative value')
            print('Enter the cost of white sugar cane per kg')
            e0_c_wsc = float(input())
    elif sweet[0]=="jaggery" or sweet[0]=="Jaggery":
        print('Enter the cost of jaggery per kg')
        e0_c_j = float(input())
        while e0_c_j<0:
            print('Cost cannot be a negative value')
            print('Enter the cost of jaggery per kg')
            e0_c_j = float(input())
elif len(sweet)==2:
    print('Enter the cost of white sugar cane per kg')
    e0_c_wsc = float(input())
    while e0_c_wsc<0:
        print('Cost cannot be a negative value')
        print('Enter the cost of white sugar cane per kg')
        e0_c_wsc = float(input())
    print('Enter the cost of jaggery per kg')
    e0_c_j = float(input())
    while e0_c_j<0:
        print('Cost cannot be a negative value')
        print('Enter the cost of jaggery per kg')
        e0_c_j = float(input())

if(len(sweet))==1 and (sweet[0]=="Sugar" or sweet[0]=="sugar"):
    e0_sub_min=0
    model.mass_Jaggery_constraint_1 = pyo.Constraint(expr = 
model.mass_Jaggery ==0)
elif (len(sweet))==1 and (sweet[0]=="Jaggery" or sweet[0]=="jaggery"):
    e0_sub_min=1
    model.mass_White_sugarcane_constraint_1 = pyo.Constraint(expr = 
model.mass_White_sugarcane ==0)
else:
    print('Enter the aimed fraction of jaggery in the sweeteners')
    e0_sub_min = float(input())
    while e0_sub_min>=1 or e0_sub_min<=0:
        print("The minimum fraction of jaggery must be between 0 and 1")
        print('Enter the minimum percentage of jaggery in the 
sweeteners')
        e0_sub_min = float(input())

#Oils
print("In that list, how many oils must be included ? (palm, sunflower, 
coconut, palm kernel, butterfat, peanut)")
nboils=int(input())
while nboils>6 or nboils<=0 :
    print("Oils are mandatory and up to five oil types can be used")
```

```
    print("In that list, how many oils must be included ? (palm, 
sunflower, coconut, palm kernel, butterfat, peanut)")
    nboils=int(input())
n=[0]*nboils
cpt=0
print("What oil(s) must be included ?")
print("type Enter after each oil")
while cpt<nboils:
    n[cpt]=str(input())
    if n[cpt]=="palm" or n[cpt]=="Palm":
        cpt=cpt+1
    elif n[cpt]=="sunflower" or n[cpt]=="Sunflower":
        cpt=cpt+1
    elif n[cpt]=="coconut" or n[cpt]=="Coconut":
        cpt=cpt+1
    elif n[cpt]=="palm kernel" or n[cpt]=="Palm kernel" or n[cpt]=="Palm 
Kernel" or n[cpt]=="palm Kernel":
        cpt=cpt+1
    elif n[cpt]=="peanut" or n[cpt]=="Peanut":
        cpt=cpt+1
    elif n[cpt]=="butterfat" or n[cpt]=="Butterfat":
        cpt=cpt+1
    else:
        cpt=0
        print("Oil(s) can oly be palm, sunflower, coconut, palm kernel, 
butterfat or peanut")
cpt=0
while cpt==0:
    for i in range (len(n)):
        if n[i]=="palm" or n[i]=="Palm":
            model.mass_Palm_oil_constraint_1 = pyo.Constraint(expr = 
model.mass_Palm_oil >=0.01)
            print('Enter the cost of palm oil per kg')
            e0_c_po = float(input())
            while e0_c_po<0:
                print('Cost cannot be a negative value')
                print('Enter the cost of palm oil per kg')
                e0_c_po = float(input())
            cpt=1
    if cpt==0:
        model.mass_Palm_oil_constraint_1 = pyo.Constraint(expr = 
model.mass_Palm_oil ==0)
        cpt=1
cpt=0
while cpt==0:
    for i in range (len(n)):
        if n[i]=="sunflower" or n[i]=="Sunflower":
            model.mass_Sunflower_oil_constraint_1 = pyo.Constraint(expr 
=  model.mass_Sunflower_oil >=0.01)
            print('Enter the cost of sunflower oil per kg')
```

```
            e0_c_so = float(input())
            while e0_c_so<0:
                print('Cost cannot be a negative value')
                print('Enter the cost of sunflower oil per kg')
                e0_c_so = float(input())
            cpt=1
    if cpt==0:
        model.mass_Sunflower_oil_constraint_1 = pyo.Constraint(expr =
model.mass_Sunflower_oil ==0)
        cpt=1
cpt=0
while cpt==0:
    for i in range (len(n)):
        if n[i]=="coconut" or n[i]=="Coconut":
            model.mass_Coconut_oil_constraint_1 = pyo.Constraint(expr =
model.mass_Coconut_oil >=0.01)
            print('Enter the cost of coconut oil per kg')
            e0_c_co = float(input())
            while e0_c_co<0:
                print('Cost cannot be a negative value')
                print('Enter the cost of coconut oil per kg')
                e0_c_co = float(input())
            cpt=1
    if cpt==0:
        model.mass_Coconut_oil_constraint_1 = pyo.Constraint(expr =
model.mass_Coconut_oil ==0)
        cpt=1
cpt=0
while cpt==0:
    for i in range (len(n)):
        if n[i]=="Palm kernel" or n[i]=="palm kernel" or n[i]=="Palm
Kernel" or n[i]=="palm Kernel":
            model.mass_Palm_kernel_constraint_1 = pyo.Constraint(expr =
model.mass_Palm_kernel_oil>=.01)
            print('Enter the cost of palm kernel oil per kg')
            e0_c_pko = float(input())
            while e0_c_pko<0:
                print('Cost cannot be a negative value')
                print('Enter the cost of palm kernel oil per kg')
                e0_c_pko = float(input())
            cpt=1
    if cpt==0:
        model.mass_Palm_kernel_constraint_1 = pyo.Constraint(expr =
model.mass_Palm_kernel_oil ==0)
        cpt=1
cpt=0
while cpt==0:
    for i in range (len(n)):
        if n[i]=="Peanut" or n[i]=="peanut":
            model.mass_Peanut_oil_constraint_1 = pyo.Constraint(expr =
model.mass_Peanut_oil >=0.01)
            print('Enter the cost of peanut oil per kg')
            e0_c_peo = float(input())
```

```
            while e0_c_peo<0:
                print('Price cannot be a negative value')
                print('Enter the cost of peanut oil per kg')
                e0_c_peo = float(input())
            cpt=1
    if cpt==0:
        model.mass_Peanut_oil_constraint_1 = pyo.Constraint(expr =
model.mass_Peanut_oil ==0)
        cpt=1
cpt=0
while cpt==0:
    for i in range (len(n)):
        if n[i]=="Butterfat" or n[i]=="butterfat":
            model.mass_Butterfat_constraint_1 = pyo.Constraint(expr =
model.mass_Butterfat >=0.01)
            print('Enter the cost of butterfat per kg')
            e0_c_b = float(input())
            while e0_c_b<0:
                print('Price cannot be a negative value')
                print('Enter the cost of butterfat per kg')
                e0_c_b = float(input())
            cpt=1
    if cpt==0:
        model.mass_Butterfat_constraint_1 = pyo.Constraint(expr =
model.mass_Butterfat ==0)
        cpt=1

print('Enter the cost of water per kg')
e0_c_w = float(input())
while e0_c_w<0:
    print('Price cannot be a negative value')
    print('Enter the cost of water per kg')
    e0_c_w = float(input())
print('Enter the cost of vanilla essence per kg')
e0_c_ve = float(input())
while e0_c_ve<0:
    print('Price cannot be a negative value')
    print('Enter the cost of vanilla essence per kg')
    e0_c_ve = float(input())
print('Enter the cost of Cremodan per kg')
e0_c_crem = float(input())
while e0_c_crem<0:
    print('Price cannot be a negative value')
    print('Enter the cost of Cremodan per kg')
    e0_c_crem = float(input())


#total milk fat = milkfat_w
```

```
expression_milkfat_w = (model.mass_Liquid_milk * e0_wf_lm)
+(model.mass_Powdered_milk * e0_wf_pm)+ (model.mass_Dairy_cream *
e0_wf_dc)+model.mass_Butterfat
#milkfat_w >= 0.02
model.expression_milkfat_w_constraint_1 = pyo.Constraint(expr =
expression_milkfat_w >= 0.02)

#total milk proteins = proteins_w
expression_proteins_w=(model.mass_Liquid_milk * e0_wp_lm)
+(model.mass_Powdered_milk * e0_wp_pm)+ (model.mass_Dairy_cream *
e0_wp_dc)
model.expression_proteins_w_constraint_1 = pyo.Constraint(expr =
expression_proteins_w >= 0.025)

#huile_w = total oils

huile_w=model.mass_Palm_oil +model.mass_Sunflower_oil+
model.mass_Coconut_oil+model.mass_Palm_kernel_oil+model.mass_Peanut_oil

#total fat = fat_w
expression_fat_w = huile_w +expression_milkfat_w

#Restrictions :
#milkfat_w <= fat_w/2
model.expression_milkfat_w_constraint_2 = pyo.Constraint(expr =
expression_milkfat_w<=huile_w)
model.expression_fat_w_constraint_1 = pyo.Constraint(expr = 0.08
<=expression_fat_w)
model.expression_fat_w_constraint_2 = pyo.Constraint(expr =
expression_fat_w <= 0.1)

#total milk-solids-not-fat fraction = msnf_w

expression_msnf_w = (model.mass_Liquid_milk*e0_wmsnf_lm ) + (
model.mass_Powdered_milk*e0_wmsnf_pm) +(
model.mass_Dairy_cream*e0_wmsnf_dc)

#Restrictions :

#msnf_w >= 0.11
model.expression_msnf_w_constraint_1 = pyo.Constraint(expr =
expression_msnf_w>= 0.11)

 #Total solids = ts_w

ts_w = expression_fat_w+ expression_msnf_w + model.mass_White_sugarcane+
model.mass_Jaggery + e0_w_em1

#Restrictions :
model.ts_w_constraint_1 = pyo.Constraint(expr = ts_w >= 0.3)
model.ts_w_constraint_2 = pyo.Constraint(expr = ts_w <= 0.36)

#liquid percentage at 5°C
```

```
expression_liquidpercentage = (model.mass_Palm_oil*.42+
model.mass_Sunflower_oil+ model.mass_Coconut_oil *.02 +
model.mass_Palm_kernel_oil*.2 + model.mass_Peanut_oil
+model.mass_Butterfat *.42)

minimumliquid=(model.mass_Palm_oil + model.mass_Sunflower_oil +
model.mass_Coconut_oil + model.mass_Palm_kernel_oil +
model.mass_Butterfat + model.mass_Peanut_oil)*.3
maximumliquid=(model.mass_Palm_oil + model.mass_Sunflower_oil +
model.mass_Coconut_oil + model.mass_Palm_kernel_oil +
model.mass_Butterfat + model.mass_Peanut_oil)*.7



model.expression_liquidpercentage_constraint_1 = pyo.Constraint(expr =
minimumliquid <= expression_liquidpercentage)
model.expression_liquidpercentage_constraint_2 = pyo.Constraint(expr =
maximumliquid >= expression_liquidpercentage)

#Level of sweetness

expression_sp = model.mass_White_sugarcane*e0_sp1+ model.mass_Jaggery
*e0_sp2


#Restrictions:

model.expression_sp_constraint_1 = pyo.Constraint(expr = expression_sp
== e0_sp_t)

model.mass_Jaggery_constraint_2 = pyo.Constraint(expr =
model.mass_Jaggery == (model.mass_Jaggery +  model.mass_White_sugarcane)
* e0_sub_min)

#Actual water content in the mix


actualwater_w = (1-(e0_wf_lm)-(e0_wmsnf_lm))* model.mass_Liquid_milk +
(1-(e0_wmsnf_dc)-(e0_wf_dc))* model.mass_Dairy_cream+(1-(e0_wmsnf_pm)-
(e0_wf_pm))* model.mass_Powdered_milk

#Required water content in the mix = requiredwater_w


requiredwater_w = 1 - ts_w
```

```
model.mass_Water_constraint_1 =
pyo.Constraint(expr=requiredwater_w==model.mass_Water+actualwater_w)

# Total cost = cost

cost = e0_totalm *((model.mass_White_sugarcane * e0_c_wsc) +
(model.mass_Jaggery * e0_c_j) + (model.mass_Liquid_milk * e0_c_lm) +
(model.mass_Powdered_milk * e0_c_pm) + (model.mass_Dairy_cream *
e0_c_dc) + (model.mass_Palm_oil * e0_c_po) + (model.mass_Sunflower_oil *
e0_c_so)+ (model.mass_Coconut_oil * e0_c_co)
+(model.mass_Palm_kernel_oil * e0_c_pko) + (model.mass_Peanut_oil *
e0_c_peo) +(model.mass_Butterfat * e0_c_b) + (e0_w_em1 * e0_c_crem) +
(model.mass_Water * e0_c_w )+ e0_c_ve*1.49/1000)

model.profit = Objective(expr = cost, sense= minimize)

results = pyo.SolverFactory('glpk').solve(model)

#Inverse of the density of the mix = inversemix_rho

inversemix_rho = ((expression_milkfat_w /
0.93)+model.mass_Palm_oil/e0_palmo_d+model.mass_Sunflower_oil/e0_so_d+mo
del.mass_Coconut_oil/e0_co_d+model.mass_Palm_kernel_oil/e0_pko_d+model.m
ass_Butterfat/e0_bf_d+actualwater_w+model.mass_Water+(expression_msnf_w
+ model.mass_White_sugarcane+ model.mass_Jaggery + e0_w_em1)/1.58)

# Required overrun = req_ov

req_ov = 100*(1/(inversemix_rho*e0_packw/1000)-1)

if (results.solver.status == SolverStatus.ok):
    print('Cost = ', value(cost))
    if value(model.mass_Water)>0:
        print('Water quantity = ', value(model.mass_Water)*100, '%,
',value(model.mass_Water)*e0_totalm,' kg')
    if model.mass_White_sugarcane()>0:
        print('White sugar cane quantity = ',
model.mass_White_sugarcane()*100, '% ,',
model.mass_White_sugarcane()*e0_totalm,' kg')
    if model.mass_Jaggery()>0:
        print('Jaggery quantity = ', model.mass_Jaggery()*100, '% ,',
model.mass_Jaggery()*e0_totalm,' kg')
    if model.mass_Liquid_milk()>0:
        print('Liquid milk quantity = ', model.mass_Liquid_milk()*100,
'% ,', model.mass_Liquid_milk()*e0_totalm,' kg')
    if model.mass_Powdered_milk()>0:
        print('Powdered milk quantity = ',
model.mass_Powdered_milk()*100, '% ,',
model.mass_Powdered_milk()*e0_totalm,' kg')
    if model.mass_Dairy_cream()>0:
        print('Dairy cream quantity = ', model.mass_Dairy_cream()*100,
'% ,', model.mass_Dairy_cream()*e0_totalm,' kg')
    if model.mass_Palm_oil()>0:
```

```
        print('Palm oil quantity = ', model.mass_Palm_oil()*100, '% ,',
model.mass_Palm_oil()*e0_totalm,'kg')
    if model.mass_Sunflower_oil()>0:
        print('Sunflower oil quantity = ',
model.mass_Sunflower_oil()*100, '% ,',
model.mass_Sunflower_oil()*e0_totalm,' kg')
    if model.mass_Coconut_oil()>0:
        print('Coconut oil quantity = ', model.mass_Coconut_oil()*100,
'% ,', model.mass_Coconut_oil()*e0_totalm,' kg')
    if model.mass_Palm_kernel_oil()>0:
        print('Palm kernel oil quantity = ',
model.mass_Palm_kernel_oil()*100, '% ,',
model.mass_Palm_kernel_oil()*e0_totalm,' kg')
    if model.mass_Peanut_oil()>0:
        print('Peanut oil quantity = ', model.mass_Peanut_oil()*100, '%
,', model.mass_Peanut_oil()*e0_totalm,' kg')
    if model.mass_Butterfat()>0:
        print('Butterfat quantity = ', model.mass_Butterfat()*100, '%
,', model.mass_Butterfat()*e0_totalm,' kg')
    print('Cremodan quantity = ', e0_w_em1*100, '%
,',e0_w_em1*e0_totalm,' kg')
    print('Vanilla essence quantity = ',e0_totalm,' mL')
    print('Density of the mix = ', value(1/inversemix_rho))
    print('Required overrun = ', value(req_ov), '%')
else:
    print('Sorry, there is no possible solution with these ingredients')
```

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