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Optimizing Process Parameters and Minimizing Ecological Impact: A Factorial Design Approach to Soap Production

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Abstract: *This study explores the optimization of process parameters and ecological impact in handmade soap production using a 2^4 factorial design with three central point repetitions. the goal was to identify the factors that influence the pH of the soap and to optimize operational conditions for producing soap with a pH below 11.5. conducted in the chemistry laboratory at the Faculty of Science and Technology, University of Zambeze, Mozambique, the experiment utilized recycled vegetable oil, sodium hydroxide (NaOH), and standard laboratory equipment. potentiometric measurements of pH were taken using a digital pH meter. Pareto analysis revealed that NaOH, oil-to-water ratio, and temperature were the most significant factors affecting pH, with an r² value of 98.60%, indicating a high model fit. response surface analysis showed that the optimal conditions for achieving a pH below 11.5 were 20g of NaOH, an oil-to-water ratio of 200/25 ml, and a temperature of 75°c. experiments 7 and 8, with a curing time of 12 days, demonstrated the best results. this research not only offers valuable insights into the optimization of soap production but also emphasizes the ecological benefits of using reused vegetable oil, promoting sustainability in the production process.*

Keywords: *Factorial Design Approach, Sustainability, Soap Production*

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I. INTRODUCTION

The ecological production of soap is a growing response to the increasing demand for sustainable practices within the industry. According to Smith et al. (2020), this approach provides environmentally friendly alternatives, promoting a potential reduction in reliance on conventional raw materials while fostering scientific advancement through the synergy of teaching, research, and community outreach.

Soap production processes are influenced by various parameters, including time, agitation, and mixing. The oil-to-water ratio, temperature, and sodium hydroxide concentration also play significant roles, highlighting the importance of identifying controllable variables. Scientifically, understanding the interplay of these factors and their impact on the final product's quality is fundamental. Traditionally, the optimization of experimental variables is conducted through univariate methods, which assess one variable at a time. However, this approach has drawbacks, such as being time-intensive and failing to evaluate the interactions between variables that influence the process under study. These limitations often result in inefficient optimization, delaying the identification of true optimal conditions, which multivariate systems can achieve more effectively (Sanghita-Basu, 2014). The factorial design stands out among various experimental design methods compared to univariate approaches. It allows the simultaneous evaluation of multiple variables with a reduced number of experimental trials (Pereira, 2018). Additional advantages include systematic work planning, resource and time efficiency, and the ability to anticipate experimental outcomes. Even with fewer trials, factorial design enables visualization of interactions among tested variables, offering a comprehensive optimization strategy.

In soap production, parameters such as excess or insufficient bases, inappropriate oil-to-water ratios, temperature conditions, and agitation/mixing times directly influence the production process. These factors significantly affect mixture homogeneity and, consequently, the product's pH. Balancing and controlling these variables is crucial to achieving consistent product quality.

Particularly, monitoring the pH of handmade soap is a critical control factor. Despite favorable macroscopic characteristics, sodium hydroxide in formulations requires adequate time for complete consumption during the saponification reaction to stabilize the pH. As observed by Pereira et al. (2012), the use of handmade soap with elevated pH can cause harmful effects, including dermal irritation, excessive removal of protective fat layers from the epidermis, and even burns due to alkalinity.

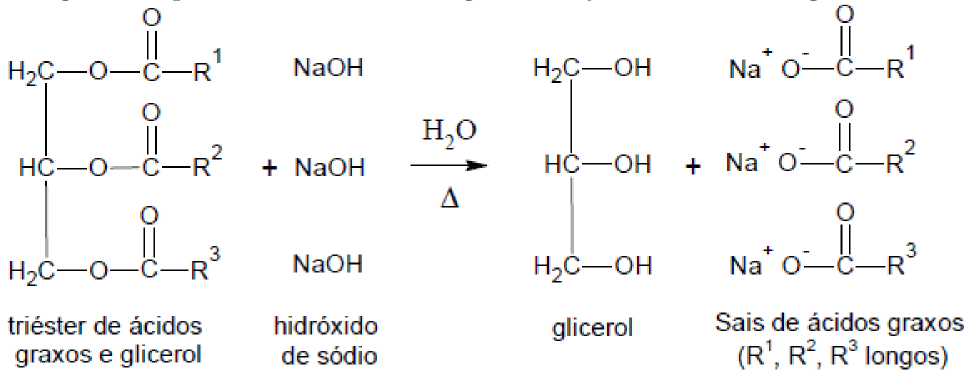
Given this context, the present study aims to apply factorial design to evaluate the influence of process parameters on the production of soap with an ecological appeal.

II. DEVELOPMENT

2.1 Saponification Reaction.

The saponification reaction, also known as alkaline hydrolysis, occurs when an ester in an aqueous solution of an inorganic base, such as NaOH, reacts to form an organic salt and alcohol. This reaction is fundamental in soap production, involving the combination of an ester derived from fatty acids with sodium hydroxide to produce an organic salt—commonly referred to as soap. Figure 1, adapted from Neto & Del Pino (2011), illustrates the molecular process of the saponification reaction.

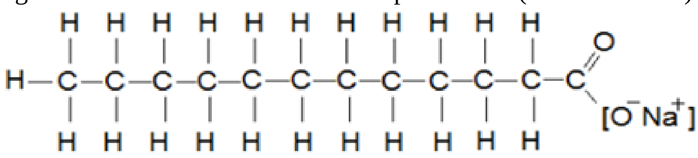
Figure 1. Saponification reaction using sodium hydroxide as an inorganic base.



Source: Neto & Del Pino (2011)

The outcome of this reaction is the formation of soap, with the general formula R-CO-ONa, where R typically represents a carbon chain containing 12 to 18 carbon atoms. The most significant structural feature of soap molecules is their amphiphilic nature: the long hydrocarbon chain has a charged (hydrophilic) end that is attracted to water, while the other end is hydrophobic and insoluble in water. Figure 2 illustrates the molecular structure of sodium laurate, a fatty acid salt, showcasing its polar and nonpolar components (Neto & Del Pino, 2011).

Figure 2. Molecular structure of a soap molecule (sodium laurate)



Source: Neto & Del Pino (2011)

2.2 Raw Materials for Soap Production.

2.2.1 Oils and Fats:

Oils and fats are widely used substances, derived from plants, seeds, and animals. Among the most well-known are soybean, cotton, peanut, sunflower, canola, sesame, flaxseed oils, and lard, which are commonly used in food preparation (Wildner & Hillig, 2012). These substances are immiscible in water and are primarily composed of a mixture of triglycerides. While oils are made up of unsaturated carbon chains, making them liquid at 20°C, fats contain saturated carbon chains, which keep them solid at the same temperature (Rabelo & Ferreira, 2008).

In food preparation, particularly in deep frying, oils and fats are used daily. In addition to providing positive modifications to sensory properties, they act as a much more efficient and faster heat transfer medium compared to cooking in water (Castellanelli, 2008). Used frying oil refers to all the residual fats, mainly of plant origin, that are utilized in frying operations intended for human consumption in the food industry, restaurants, and households. The increase in temperature during frying, exceeding 200°C, causes the degradation of triglycerides through hydrolytic and oxidative reactions, known as rancidification. This results in the formation of polar compounds that alter the oil's characteristics, making it darker, more viscous, more acidic, and producing an unpleasant odor commonly referred to as rancidity, which necessitates the disposal of these oils and fats (Reis et al., 2007). Improper disposal of used cooking oil can have detrimental effects on the environment. In this context, repurposing this oil for eco-friendly soap production contributes to environmental issues and represents an opportunity for income generation (Leal et al., 2010).

2.2.2 Sodium Hydroxide (NaOH):

According to Vitori and Frade (2012), sodium hydroxide is a strong inorganic base with a high capacity to accept protons. When it reacts with water and alcohol, it releases OH- ions, which dissociate easily in solution. When in contact with fats and oils, it produces the soap used for cleaning. The physical and chemical properties of sodium hydroxide are detailed in Table 1.

Table 1. **Physical-Chemical Properties of Sodium Hydroxide**

Chemical Formula	NaOH
Molecular Weight	40,00
Melting Point	318 ºC
Boiling Point	1390 ºC
Specific Gravity (20ºC/20ºC)	2,13 g/cm³
Color	White Scales
Solubility in Water (20ºC)	109g/ 100g water

Source: Carbocloro (2015)

According to Neves (2009), sodium hydroxide is the primary saponifying agent due to its wide availability in the market, low cost compared to other agents, high alkaline strength, and suitable hardness and solubility characteristics for commercialization in *bar* or chunk form. However, according to Benedito and Minatti (2014), handling NaOH requires special care. It should be done in well-ventilated areas or with local ventilation/exhaust systems, and the use of Personal Protective Equipment (PPE), such as gloves, rubber aprons, respiratory protection, and goggles, is essential. Additionally, stainless steel materials should be used, and contact with metals such as aluminum, zinc, tin, and their alloys should be avoided, as they react with the compounds in the solution.

2.2.3. Water:

Water plays a fundamental role in soap production, as it emulsifies fats during the process, facilitating their combination with alkalis and enhancing saponification. However, not all waters are suitable for soap manufacturing. Hard waters, which primarily contain dissolved calcium and magnesium salts (Ca2+ and Mg2+), must be chemically treated. This can be done using lime and sodium carbonate together, sodium carbonate alone, or caustic soda. The use of hard water favors the ion-exchange reaction of sodium or potassium ions, present in the soap molecule, with calcium or magnesium ions in the aqueous solution. Since the salts formed are insoluble, precipitate forms, preventing the soap from performing its cleaning function (Del Pino & Neto, 2011).

2.2.4. Co-ingredients:

Co-ingredients are products used in soap formulations to impart important characteristics to the product or provide special properties, although they are not essential. Additionally, some of these products are used as simple fillers to minimize production costs. Among the compounds classified as co-ingredients are sodium chloride, sodium and calcium carbonates, silicates, phosphates, sugar, starch, kaolin, antioxidants, bleaching agents, and others (Neves, 2009).

2.2.5. pH (Hydrogen Ion Potential):

As a concept proposed by Sorensen in 1909, pH means 'power of hydrogen,' and it describes the predominant acidic or basic character in an aqueous medium, with values on a scale from 0 to 14. An aqueous medium is considered acidic with a pH of 0 to 7, basic from 7 to 14, and neutral at pH 7 (PEDROSA, 2015). The salt produced by the saponification reaction generally has a basic character, resulting from the reaction between a strong base (NaOH) and a weak acid (fatty acid).

Alkaline soaps are better at removing dirt due to interactions with dirt molecules, but excessive alkalinity can make them unsuitable for use, turning their action caustic (Neto & Del Pino, 2011). Bar soaps should have a maximum pH of 11.5 for cleaning purposes, while personal hygiene soaps should have a maximum pH of 10.5 (WHO, 2012). Strongly alkaline soaps have a dehydrating and irritating potential for human skin, so they are not recommended for use (MENDES et al., 2016).

2.3 **Ecological Appeal: Recycling Frying Oil Residues**

The implementation of selective collection, as highlighted by Rabelo and Ferreira (2008), also contributes to the separation of residual oil that could otherwise be discarded improperly into the environment. Thus, raising awareness enables proper disposal, contributing to environmental balance. According to Heinzen and Junglos (2013), waste should be treated with greater care for the preservation of life on the planet, not viewed as the end of a cycle but as the beginning of another. The authors adopt the concept of the 3Rs: Reduce, Reuse, and Recycle. Humans should consume less, reuse products multiple times, and recycle materials to create something new. This concept has generated the idea of sustainability, which is becoming increasingly relevant.

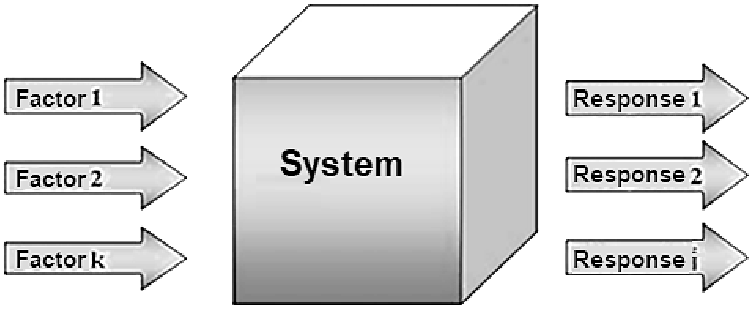
2.4 **Factorial Planning**

Experimental planning is a powerful tool for studying the combined effect of several factors on a response variable of interest. A widely recognized technique is factorial planning, where k factors or variables are involved, each at different levels. The simplest case occurs when each factor k is present at only two levels. When experimenting with k factors at two levels, 2^k observations of the response variable are made, known as a 2^k factorial experiment (Montgomery, 2015).

Figure 3 illustrates the scheme of several factors k acting in an experiment, resulting in responses R1, R2, ..., Rj. The system operates with an unknown function over the input variables (the factors), producing the observed responses. Thus, the goal of experimental planning is to discover this function or obtain a relevant approximation to it, allowing for the selection of the best execution conditions for the system.

Factorial planning is widely used in basic and technological research, classified as a simultaneous method, in which the relevant variables in the response are evaluated at the same time (DRUMOND, 2008). In this method, all treatments composing the experimental matrix are performed by the team responsible for the activity. For example, consider an experiment with two factors (A and B), each with levels for factor A and B levels for factor B. Thus, there are ab test combinations in this experiment. The planning matrix for the two-factor factorial experiment at levels a and b is represented in Table 3. This organization also describes the general case of the two-factor factorial experiment for an observed response, when factor A is at the i-th level (i = 1, 2, ..., a). It is important to highlight that the ABn observations of the experiment can be performed randomly (GALDÁMEZ, 2002).

Figure 3. **System representing a function linking the factors to the responses.**



Source: Da Silva (2008)

III. EXPERIMENTAL PROCEDURE

3.1 **Materials and Methods**

The experimental development was conducted in the Chemistry Laboratory at the Faculty of Science and Technology of the University of Zambeze, located in Mozambique, on the African continent. Various materials, reagents, glassware, and equipment were used, including reused vegetable oil (from frying), sodium hydroxide in flakes, pH meter brand PH8+ DHS, electric heating plate brand MS7-H550-S, digital analytical balance, magnetic stirrer, 600-milliliter glass beaker, 250-milliliter glass beaker, filter paper, and watch glass.

Focusing on the pH evaluation, this test aims to determine the hydrogen potential of a soap sample solution by potentiometry. This is done by determining the potential difference between two electrodes — the reference electrode and the measuring electrode — immersed in the analyzed sample (ANVISA, 2012).

Table 5. pH stabilized soap measurements

Experiments	pH_1	pH_2	pH_3	Average
1	10,09	10,04	10,07	10,07
2	10,04	10,08	10,01	10,04
3	10,39	10,40	10,37	10,39
4	10,53	10,57	10,55	10,55
5	10,97	10,93	10,88	10,93
6	11,09	11,06	11,10	11,08
7	10,74	10,70	10,70	10,71
8	10,82	10,89	10,90	10,87
9	12,07	12,03	12,05	12,05
10	12,18	12,20	12,17	12,18
11	11,03	11,00	11,06	11,03
12	11,39	11,35	11,40	11,38
13	12,59	12,60	12,59	12,59
14	12,72	12,80	12,82	12,78
15	11,28	11,15	11,30	11,24
16	11,32	11,28	11,26	11,29
17C	11,15	11,24	11,17	11,19
18C	11,08	11,19	11,10	11,13
19C	10,92	10,89	11,00	10,94

Source: Authors (2024)

Table 2. Factors and levels used in the full factorial design (24)

Variables	Levels		
	Lower (-1)	**Central (0)**	**Superior (+1)**
1. Mixing time (min)	30	40	50
2. Oil/water ratio (ml)	200/50	200/33	200/25
3. Temperature (°C)	25	50	75
4. NaOH (g)	20	30	40

Source: Authors (2024)

Table 3. Coded levels of the experimental design

Experimental Trials	Mixing time (min)	Oil/water ratio (ml)	Temperature (ºC)	NaOH (g)
1	-1	-1	-1	-1
2	1	-1	-1	-1
3	-1	1	-1	-1
4	1	1	-1	-1
5	-1	-1	1	-1
6	1	-1	1	-1
7	-1	1	1	-1
8	1	1	1	-1
9	-1	-1	-1	1
10	1	-1	-1	1
11	-1	1	-1	1
12	1	1	-1	1
13	-1	-1	1	1
14	1	-1	1	1
15	-1	1	1	1

16	1	1	1	1
17C	0	0	0	0
18C	0	0	0	0
19C	0	0	0	0

Source: Authors (2024)

Table 4. Real values of the experimental design 24 plus three central points.

Experimental Trials	Mixing time (min)	Oil/water ratio (ml)	Temperature (ºC)	NaOH (g)
1	30	200/50	25	20
2	50	200/50	25	20
3	30	200/25	25	20
4	50	200/25	25	20
5	30	200/50	75	20
6	50	200/50	75	20
7	30	200/25	75	20
8	50	200/25	75	20
9	30	200/50	25	40
10	50	200/50	25	40
11	30	200/25	25	40
12	50	200/25	25	40
13	30	200/50	75	40
14	50	200/50	75	40
15	30	200/25	75	40
16	50	200/25	75	40
17C	40	200/33	50	30
18C	40	200/33	50	30
19C	40	200/33	50	30

Source: Authors (2024)

The pH values were determined using the digital device brand PH8+DHS, model 5040-0203D. The procedure for digitally measuring the pH of the product was as follows: initially, 10 grams of the soap sample were dissolved in 100 ml of water in a 250 ml beaker, using a heating plate to facilitate the dissolution. After cooling the solution to calibrate the pH meter, the reading was performed according to the method recommended by Coabianco (2015). Due to the manual homogenization of the mixture, pH measurements were taken in replicates (three measurements of the same sample) to check for variations in the values. Table 5 describes the experimental measurements for pH stabilities. Regarding the analysis of the results obtained, a full two-level factorial design with four factors was carried out, totaling 16 experiments. In addition, three repetitions at the central point were added for the estimation of pure error, resulting in a total of 19 experiments. The procedure for formulating the full factorial design began with screening the main variables that influence the soap-making process, such as agitation and mixing time, oil/water ratio (keeping the same oil amount), temperature, and NaOH amount, to determine the response variable of interest — pH. Table 2 presents the actual levels of the independent variables, while Tables 3 and 4 describe the variations in the reaction média, as proposed.

IV. RESULTS AND DISCUSSIONS

4.1 Experiment Responses

From the matrix presented, the tests of the experimental design proposed in this study were conducted. The obtained values for the response variable pH after the drying of the handmade soap are detailed in Table 6. Based on the results presented in Table 6 and using the Statistica 7.0 software, the effects of each parameter in the handmade soap manufacturing process were calculated. An analysis of the influence of these parameters on the dependent variable – the pH of the soap – was then conducted. To this end, it was necessary to determine which variables were statistically significant, which was visualized through a Pareto diagram (Figure 4).

The Pareto diagram associates the effects of each variable individually and their two-by-two interactions, showing that a variable's effect on pH is significant if the corresponding bar exceeds the red line, where the significance level is set at 95%. This graph was used to demonstrate the effects of the studied variables—mixing time, oil/water ratio, temperature, and NaOH amount—and their interactions on the soap's pH. It was observed that the variable that most influenced the soap's pH was NaOH.

A possible explanation for this is that NaOH is a very strong base that reacts with a weak acid. Since this variable has a positive response (20.19), it indicates that increasing the NaOH content increases the soap's pH. After NaOH, the interaction between the oil/water ratio and NaOH was the next most influential factor on the pH, surpassing the individual effects of the oil/water ratio. The oil/water ratio presented a negative response (-9.71), indicating that an increase in the oil/water ratio would lead to a decrease in pH.

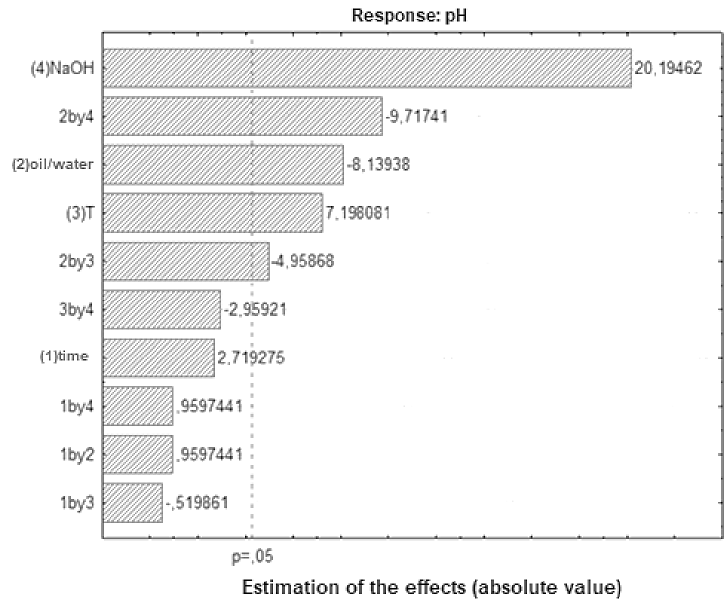
Temperature also had a significant influence on the soap's pH. The positive effect (7.19) indicates that this variable, at its maximum level (75°C), will increase in pH value. Among the four studied variables, mixing time had the least impact on pH and was not statistically significant at the 95% confidence level

Table 6. Experimental Design with Matrix of Real Independent Variables and Response Variable pH

Experimental Trials	Mixing Time (min)	Oil/Water Ratio (ml)	Temperature (°C)	NaOH (g)	Response pH
1	30	200/50	25	20	10,07
2	50	200/50	25	20	10,04
3	30	200/25	25	20	10,39
4	50	200/25	25	20	10,55
5	30	200/50	75	20	10,93
6	50	200/50	75	20	11,08
7	30	200/25	75	20	10,71
8	50	200/25	75	20	10,87
9	30	200/50	25	40	12,05
10	50	200/50	25	40	12,18
11	30	200/25	25	40	11,03
12	50	200/25	25	40	11,38
13	30	200/50	75	40	12,59
14	50	200/50	75	40	12,78
15	30	200/25	75	40	11,24
16	50	200/25	75	40	11,29
17C	40	200/33	50	30	11,19
18C	40	200/33	50	30	11,13
19C	40	200/33	50	30	10,94

Source: Authors (2024)

Figure 4. Pareto diagram of the standardized effects for the response variable pH

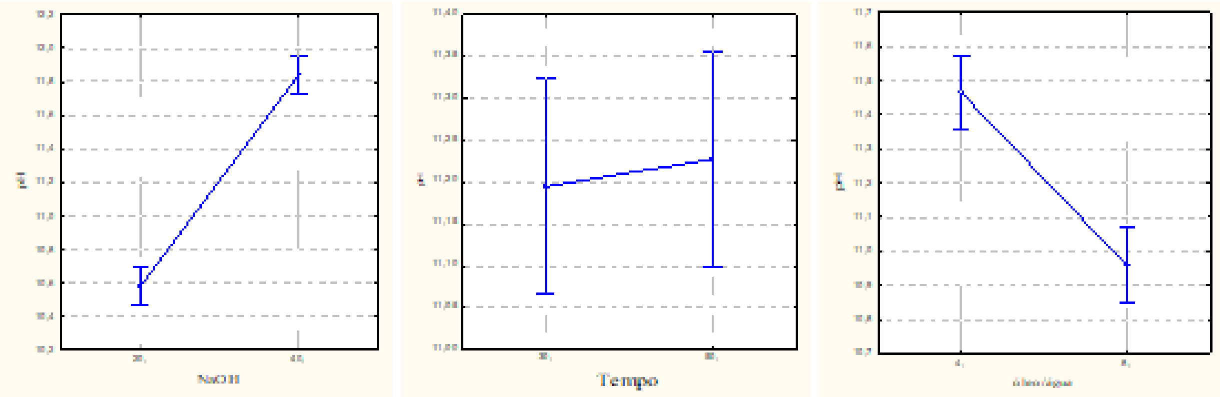


Source: Authors (2024)

4.2. Graphs of Effects

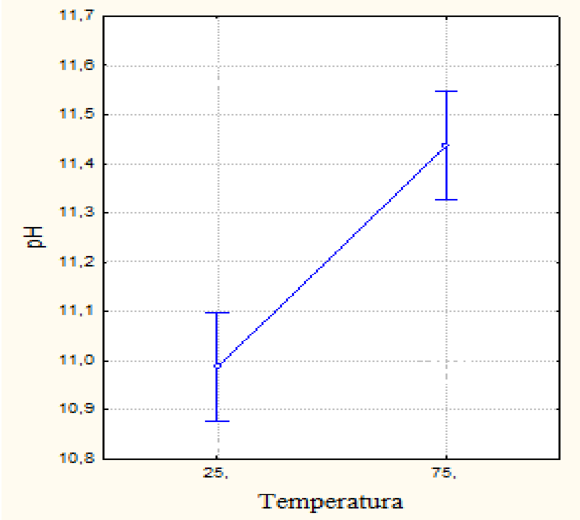
To facilitate the understanding of these results, Figure 5 graphically presents the main effects, showing how the response variable (pH) changes when the factors move from the low (-) to the high (+) level, or vice versa. Additionally, Figure 6 illustrates the main effects of the factors temperature and mixing time. It is observed that the factors considered statistically significant (NaOH, oil/water ratio, and temperature) show a significant variation in the response variable (average pH) between the analyzed levels, while the variation in the mixing time level causes virtually no significant change in the response.

Figure 5. **Main effects of the NaOH factor and oil/water ratio**



Source: Authors (2024)

Figure 6. Main effects of the temperature and mixing time factors.

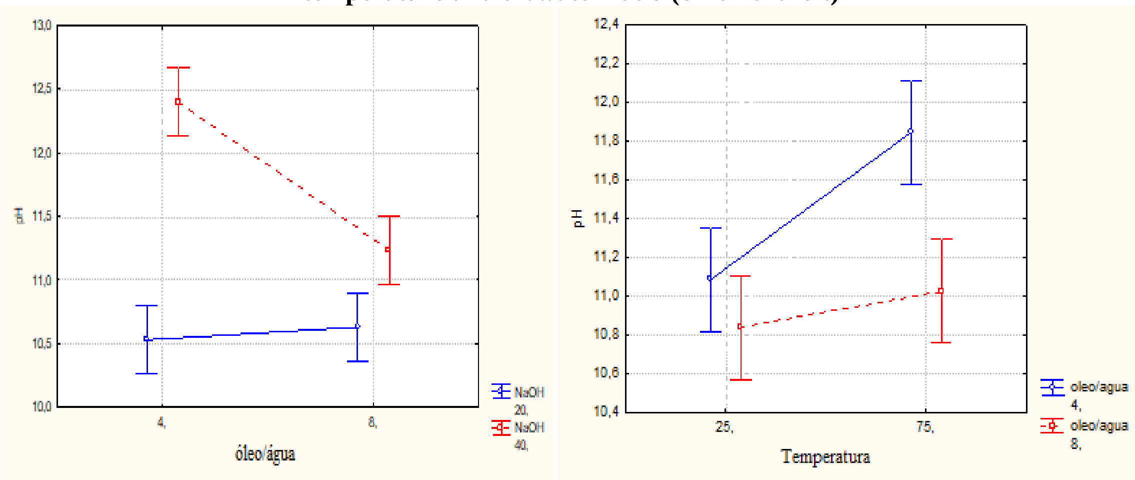


Source: Authors (2024)

4.3 Interaction Effects

As illustrated in Figure 7a, the variation in the oil/water ratio has less influence when the amount of NaOH is at the low level, highlighting the importance of controlling the amount of NaOH. In Figure 7b, it is observed that, with an oil/water ratio of 200/25, the pH value is virtually the same for both temperatures. However, with an oil/water ratio of 200/50, the increase in pH is directly related to the increase in temperature. The response highlighted in the Pareto diagram (Figure 10) is corroborated when examining the effect calculations, presented with the significant variables and interactions highlighted in red. According to Santos et al. (2009), a high effect value indicates that a small change in the independent variable results in a significant change in the dependent variable, making it an important factor in the process. The 'p' column denotes the probability that an independent variable has no effect on the dependent variables. In other words, low 'p' values indicate a high probability that a change in the independent variable will cause a significant change in the dependent variable (Santos et al., 2009). The analysis of the 'p' values confirms that, for a 95% significance level, the variables NaOH, oil/water ratio, temperature, and the interactions between oil/water ratio and NaOH, as well as between temperature and oil/water ratio, are statistically significant for the pH of the handmade soap (Table 7).

Figure 7. Interaction effects of oil/water ratio and NaOH (a - on the right); Interaction effects of temperature and oil/water ratio (b - on the left)



Source: Authors (2024)

Considering the significant effects at a 95% confidence level, we propose the model described by Equation 1. The application of this mathematical equation expresses the relationship between the variables of interest, identifying the factors that influence the outcome and providing guidelines for their resolution.

Equation 1: The relationship between variables of interest (significant effects at a 95% confidence level)

$$\mathrm{pH} = 11{,}18964 - 0{,}50881 * \mathrm{R} + 0{,}45000 * \mathrm{T} + 1{,}26250 * \mathrm{C} - 0{,}31000\mathrm{R} * \mathrm{T} - 0{,}60750\mathrm{R} * \mathrm{C}$$

Where: R - Oil/Water Ratio; T - Temperature; C - NaOH.

The experimental results for the pH of the soap, obtained during the execution of the 24-factorial design, were subjected to analysis of variance (ANOVA) to evaluate the model obtained (Table 8). Thus, by comparing the calculated F-value for the regression of each variable and its interactions with the tabulated F-value (F Table = 19.41), as presented in the ANOVA table for pH with a 95% confidence level, we observe that the factors (NaOH, temperature, and oil/water ratio) and their interactions (oil and temperature ratio) have a calculated F-value greater than the tabulated F-value and p values ≤ 0.05, indicating a significant regression, i.e., they influence the response.

Table 7. Effect calculations for the pH of the handmade soap.

Factors	Regression Coefficients	Pure Error	t(2)	P	95% Conf. Limit (-)	95% Conf. Limit (+)
Mean/Interaction	5,643223	0,760917	7,41635	0,017700	2,369262	8,917184
Mixing Time	-0,006250	0,015648	-0,39942	0,728202	-0,073577	0,061077
Oil/Water Ratio	0,423470	0,089355	4,73918	0,041755	0,039006	0,807934
Temperature	0,041300	0,007721	5,34892	0,033220	0,008078	0,074522
NaOH Quantity	0,160750	0,017871	8,99499	0,012135	0,083857	0,237643
Interaction Time - Oil/Water	0,001500	0,001631	0,91946	0,454921	-0,005519	0,008519
Interaction Time - Temperature	-0,000065	0,000131	-0,49804	0,667829	-0,000627	0,000497
Interaction Time - NaOH	0,000300	0,000326	0,91946	0,454921	-0,001104	0,001704
Interaction Oil/Water - Temperature	-0,003100	0,000653	-4,75053	0,041568	-0,005908	-0,000292
Interaction Oil/Water and Temperature	-0,015188	0,001631	-9,30950	0,011343	-0,022207	-0,008168
Interaction Temperature and NaOH	-0,000370	0,000131	-2,83499	0,105159	-0,000932	0,000192

Source: Authors (2024)

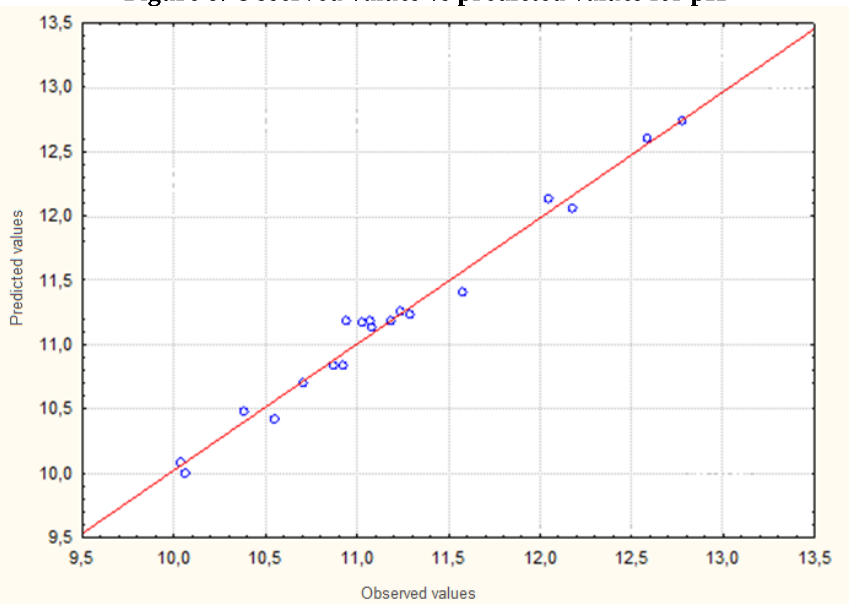
Table 8. ANOVA results for pH of handmade soap. F (12, 2; 0.95) = 19.41 (Tabled)

Efeitos Estimados; R^2= 0,98702; Ajuste: 0,97079; MQ Erro Puro = 0,0170333					
Variation Source	**Sum of Squares**	**Degrees of Freedom**	**Mean Square**	**F Calculated**	**P**
Mixing time	0,1156	1	0,1156	6,7867	0,1212
Oil/Water ratio	1,0349	1	1,0349	60,7586	0,0160
Temperature	0,8100	1	0,8100	47,5538	0,0204
NaOH amount	6,3752	1	6,3756	374,3026	0,0027
Interaction Time and Oil/Water	0,0144	1	0,0144	0,8454	0,4549
Interaction Time and Temperature	0,0042	1	0,0042	0,2480	0,6678
Interaction Time and NaOH	0,0144	1	0,0144	0,8454	0,4544
Interaction Oil/Water and Temperature	0,3844	1	0,3844	22,5675	0,0415
Interaction Oil/Water and NaOH	1,4762	1	1,4762	86,6668	0,0113
Interaction Temperature and NaOH	0,1369	1	0,1369	8,0372	0,1051
Lack of fit	0,1023	6	0,0170	1,0009	0,5778
Pure Error	0,0341	2	0,0170		
Total Sum	10,5034	18			

Source: Authors (2024)

Figure 8 illustrates the observed values versus the predicted values for pH. The evaluation of the model can also be done through the graph of predicted values versus observed values. The predicted values by the model are represented by a straight line, while the observed values are represented by points. It is observed that the model has a good fit quality because most of the values are evenly distributed around the straight line, and the distribution of positive and negative deviations is random, indicating that they occur in the same proportion.

Figure 8. Observed values vs predicted values for pH



Source: Authors (2024)

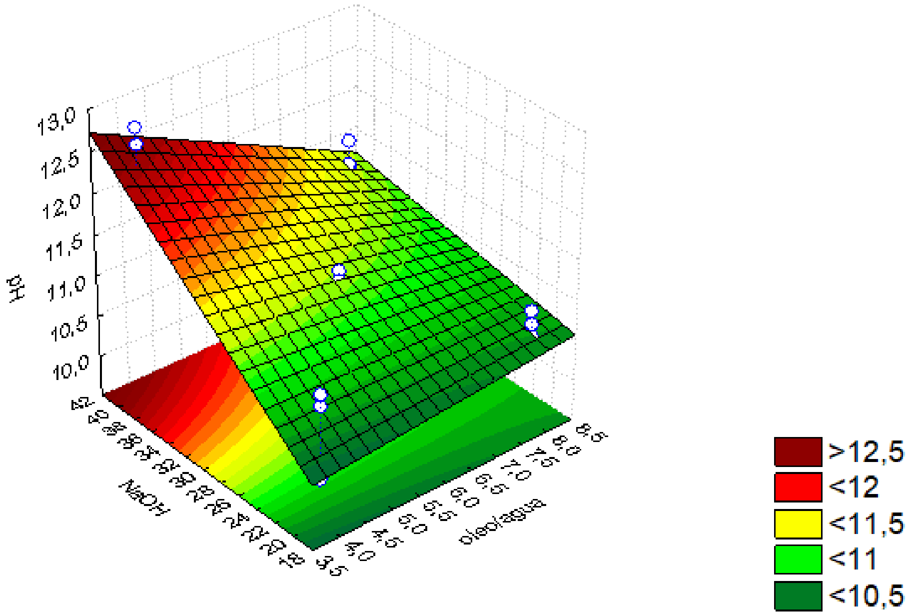
In practical terms, it can be stated that the model has a good fit, as the regression was significant, and the lack of fit was not significant. This means that most of the variation in the mean was explained by the regression equation, while the remainder was attributed to the residuals. The majority of the residual variation was due to experimental error, not to the lack of fit, which is directly related to the model. The obtained coefficient of determination was 0.9870, meaning that 98.70% of the variation in the pH of the handmade soap can be explained by the variation in the independent variables: sodium hydroxide, temperature, and oil/water ratio, as well as by the interactions between oil/water ratio and NaOH, and between oil/water ratio and temperature (model).

4.4 Response Surface Analysis

Essentially, response surface methods help explore the relationships between variables and quantitative experimental factors. After identifying significant factors, these methods enable the optimization of the experiment, meaning finding the ideal levels that will produce the best-desired response, representing the optimal region on the surface defined by the factors.

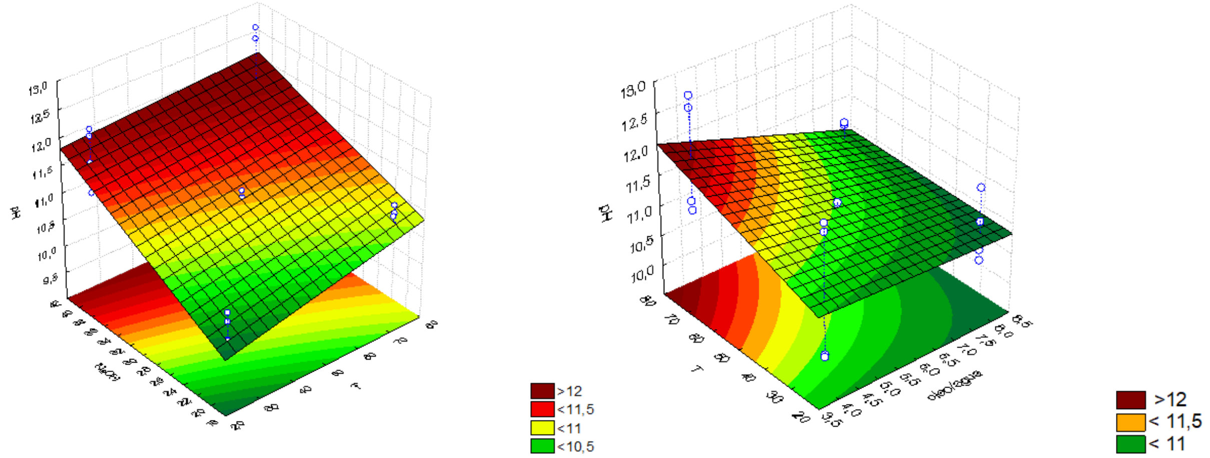
When analyzing the response surface for the pH of the soap (Figure 9), it is observed that NaOH has a more significant influence than the oil/water ratio variable. This occurs because the oil/water ratio remains almost constant when the operating conditions involve low quantities of NaOH. However, as the amount of NaOH increases, the oil/water ratio begins to have a significant effect on the response. Therefore, to achieve a pH below 11.5, the ideal operating conditions were 20g of NaOH and an oil/water ratio of 200/25.

Figure 9. Response Surface for pH as a function of the NaOH and oil/water factors.



Source: Authors (2024)

Figure 10. Response Surface for pH as a function of NaOH and temperature factors (a - on the left); Response Surface for pH as a function of temperature and oil/water factors (b- on the right)



Source: Authors (2024)

The analysis of Figures 10a and 10b reveals interesting patterns regarding the influence of NaOH, temperature, and the oil/water ratio on the pH of the soap. In Figure 10a, we can observe a strong relationship between the increase in soap pH and the change in the NaOH factor level at high temperatures. When there is a low amount of NaOH, the influence of temperature is less pronounced and only becomes noticeable at its maximum levels. However, when a low amount of NaOH and high temperatures are used, minimal pH values are obtained. In Figure 10b, it can be seen that with higher oil/water ratios, changing the temperature did not significantly affect the pH, indicating that the variation in temperature had no significant impact on pH. However, at lower oil/water ratios, there was a positive influence on pH, where increasing temperature resulted in an elevation of pH. This suggests that the influence of the oil/water ratio variation was not significant at low temperatures, but at high temperatures, it had a positive effect, reaching maximum pH values at low oil/water ratios and high temperatures.

V. CONCLUSION

Based on the results from the 2^4 factorial design with three central point repetitions, the most significant variables affecting the pH of handmade soap were identified. Pareto analysis indicated that sodium hydroxide (NaOH), oil/water ratio, and temperature were statistically significant factors influencing pH at a 95% confidence level. The linear model provided an excellent fit to the data, with an R^2 value of 98.60%, indicating that the model could explain 98.60% of the observed variance in pH. This high R^2, along with the statistical significance of the model, confirms its reliability for predictive purposes.

The response surface analysis revealed that the optimal operational conditions for achieving a pH below 11.5 were 20g of NaOH, an oil/water ratio of 200/25 ml, and a temperature of 75°C. Based on these findings, the best experimental conditions were observed in experiments 7 and 8, with a curing time of 12 days. These conditions proved to be the most effective in achieving a balanced pH, ensuring the production of soap suitable for use.

In conclusion, the study provides valuable insights for optimizing the handmade soap production process, enabling the production of soaps with an appropriate pH for consumer safety and quality. The results offer clear guidance for achieving the desired pH values and contribute to more efficient and consistent soap manufacturing practices.

Conflict of interest

There is no conflict to disclose.

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