Optimization of a Functional Beverage Formulation Using a Constrained Mixture Design with Multiple Responses

Abstract

Functional beverages refer to a relatively new and expanding market segment appearing that goes beyond simple nutrition but contains some beneficial ingredients. This study employs a constrained mixture design to optimize a functional beverage's formulation by systematically analyzing the interactions between three key ingredients: fruit juice blend, low fat probiotic yogurt and a functional ingredient. Based on D-optimal experimental design the research mimics response across various factors such as taste, texture, perceived health benefits. To assess the impact of the ingredient proportions, a second-degree mixture model was used, while the levels of the ingredient constraints were set at 40-70% for fruit juice blend, 20-40% for probiotic yogurt, and 10-30% for the functional ingredients. Further quantitative analysis in this study confirmed that fruit juice blend was statistically significant in all the response variables as the most influential factor controlling the treatment while probiotic yogurt also had strong but slightly lesser influence. Desirability functions used in the optimization process yielded the maximal proportion of the fruit juice blend of 0.7, probiotic yogurt 0.5, and functional ingredient 0.5. This work offers scientific approach to creating functional beverages with enhanced sensory qualities to match enhanced health properties, solving a current gap in techniques for extended food science in beverage development.

Keywords: D-optimality experimental design, second-degree mixture model, optimization process, constrained mixture design

1. Introduction

Functional beverages referring to the designed food products meant for specific consumer health needs are emerging very strongly in the food and beverage industry. This growth is driven by higher levels of consumer concern over Wellness products that are healthy for the body through natural substances such as vitamins, minerals, antioxidants, and bioactive compounds (Galvan et al., 2021). The unique requirements of this market put pressure on the manufacturers to create the beverages that will not only be healthy but also desirable for consumers, thus, the requirement for the accurate balancing of the respective formulas. To strike this balance, researchers use what is known as mixture experiments, which is especially beneficial when ingredient ratios, not amounts, determine the properties of the end product (Shiby et al., 2013).

In particular when dealing with functional beverages the ability to blend several ingredients most of which have different flavour, texture and functionality is very critical to meet both consumer preferences and health benefits. Mixture experiments provide a systemic technique for analysing and predicting the performance of the ratios of the ingredients on multiple characteristics such as flavor, nutrition, shelf-life etc. For instance, mixture designs have been implemented successfully for the development of beverages such as chocolate-flavored, peanut–soy drinks; blends containing Hibiscus sabdariffa for antioxidant properties (Ogundele et al., 2016); and energy drinks from whey and fruit extracts (Shiby et al., 2013; Deshpande et al., 2008). These kinds of studies illustrate the possible of using mixture designs as a more precise tool of adjusting complicated recipes, since it takes into consideration the interactions of the components, thus directing the formulation process to improve results.

Functional beverage formulation is usually challenged by one or more design factors which means that in the course of formulating functional beverages, more than one acceptable characteristic usually has to be considered at the same time, hence the process is referred to as multi objective optimization. For example, Castro et al. (2003) used this strategy in fractional optimality of protein mixtures. Lawless et al. (2013) used a mixture design to optimise the ratio of black cherry, Concord grape, and pomegranate juices that would be preferred by consumers. Some have been developed to meet a taste appeal, appearance and nutritional value, as done by Akonor (2020) in fruit juice cocktail and Ban et al. (2010) in black ginger beverage. When modeling multiple responses, researchers can solve conflicting goals, which is critical in formulating products that meet the multitude of requirements of the functional beverage segment.

This paper uses a constrained mixture design to model and optimize the formulation of a functional beverage, with focus on both sensory and functional properties constraints by ingredients. It is through such an experimental setup that the present study will be able to determine optimal formulation that would aptly fit consumer health concerns and market trends about beverages, and integrate such knowledge in the existing paradigms on progressive food science methodologies in the development of functional beverages (Bezerra et al., 2010; Baú et al., 2013).

2. Methodology

2.1. Experimental Design

The functional beverage formulation includes three components of mixtures. The first variable is the fruit juice blend (X_1); it can be apple, grape, etc and is the major ingredient for the flavour and the nutritional complement of the soda. In the formulation of the canine food, there is a variation of the proportion of fruit juice which ranges from 40 % to 70%. The second ingredient, that is probiotic yogurt (X_2), adds functional characteristics by containing the probiotics which help in digestive health, and also in giving the product the right texture. A probiotic yogurt fraction is different and ranges from 20% to 40%. The third aspect is functional ingredient (X_3) which could be plant protein, fibre or other functional compound. This ingredient contributes to other health gains including; enhancement of bowel movements, boosting energy, and creating a sense of wellbeing. The proportion of the functional ingredient is within a fairly narrow range and can not be less than 10% or more than 30%. These constraints on the ingredient proportions guarantee that one is still able to design a viable formulation even as one seeks to make changes for specific sensory or functional effects

2.2. Response Variables

Evaluating the success of the beverage formulation, three response variables were considered: first the product taste (Y_1), second the product texture (Y_2) and third the health benefit perceived from the product (Y_3). These variables are each given a number on a range of 1–10 quantitatively relative to the quality or perception perception: with 1 representing poor and 10 representing an ideal or highly positive characteristic. Y_1 captures the general preference for the taste of the product since taste is an important determinant of the consumers' acceptance. Texture (Y_2) assesses the feeling of the product associated with the appearance, viscosity and palatability of the product when it is being consumed as a beverage. Thirdly, the perceived health benefit (Y_3) assesses consumer belief about the functional benefits of the product, factors that make it unique and superior to other similar products. These three response variables give the complete picture of how the mixture components influences the sensory and functional properties of the beverage.

2.3. Experimental Design Selection

To capture these relationships, an appropriate experimental design known as D-optimal experimental design is used. D-optimal design was selected as it offers the least determinant of covariance matrix, offering the best estimates for the regression model with fewer runs than the other designs. This makes a choice of experimental points as effective since it would produce adequate data for the modeling of how the proportions of ingredients would affect the efficiency of the beverage. It is especially appropriate in mixture experiments where the proportion of components or constituents is limited enabling adequate search of a higher order design space.

2.4. Data Collection Process

The data for this study is gathered through simulation. In this approach, response data for the different combinations of the ingredient proportions, due to the stated constraints, is produced. The taste, texture, and perceived health-benefit/output simulated responses are computed employing an assigned model that substantiates plausible fluctuation in customer appraisals in terms of the ingredients ratio. The simulation therefore mimics actual response levels to each ingredient incorporating the individual impacts and interactional impacts. By using this simulation process one does not have to form the mixture physically and test it and therefore saves a lot of time and money yet at the same time you get to study the behavior of the mixture as it is changed over the stated ranges.

2.5. Statistical Analysis Methods

The data is analyzed using a second-degree mixture model in order to determine the best formulation of the components. The linear and non-linear effects of the ingredients and their interaction with the response variables are also displayed in the model.. The equation for the second-degree mixture model is as follows:

$$Y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \varepsilon$$

Where:

- Y represents the response variable (Y_1, Y_2, or Y_3),
- x_1, x_2, and $x_3$are the proportions of the fruit juice blend, probiotic yogurt, and functional ingredient, respectively,
- β_1, β_2 and $\beta_3$are the linear coefficients for the ingredients,
- β_{12}, β_{23} and β_{13} are the interaction coefficients for ingredient pairs,
- $\varepsilon$is the error term representing random variations.

This model makes it possible to evaluate how the proportion of the ingredients (x_1, x_2, x_3) affect the responses. The coefficients for the model equations are obtained using least squares regression, and and the significance of each term in the model is determined through analysis of variance (ANOVA).

2.6. Model Validation and Optimization

After the model is fitted, the optimization step runs the desirability function to obtain ingredient proportions which would yield maximum desirability. The desirability function integrates multiple responses into one annotated value by turning each answer into a desirability value between 0 and 1 with 1 being the most desirable. From these individual scores we can compute the total desirability score. Furthermore, the sensitivity analysis is carried out in order to evaluate the effect of the variations of certain ingredient ratios on traits of the final product and to determine the key ingredients and their concentration. Model diagnostics such as residual analysis and goodness-of-fit measures are performed to verify the accuracy and adequacy of the model, ensuring that it captures the underlying relationships between the components and response variables.

3. Results and Discussion

3.1 Summary Statistics

The summary statistics in Table 1 reveal insights into the functional beverage formulation experiment. For the mixture components, X1 (fruit juice blend) ranges from 0.481 to 0.691, with a mean of 0.602, indicating that fruit juice blend constitutes a significant portion of the beverage. X2 (probiotic yogurt) varies from 0.230 to 0.454, with a mean of 0.339, suggesting moderate yogurt content. X3 (functional ingredient) shows the least variation, ranging from 0.146 to 0.278, with a mean of 0.215. Regarding response variables, Taste ranges from 2.992

to 4.401, with a mean of 3.748, indicating generally positive taste evaluations. Texture has lower values, ranging from 2.359 to 3.565, with a mean of 3.123, suggesting room for improvement. Health Benefit shows consistently positive scores, ranging from 3.169 to 4.586, with a mean of 4.038, indicating that the formulations are perceived as beneficial to health.

Table 1: Descriptive Statistics of Functional Beverage Formulation Components and Responses

Variable	**Minimum**	**Maximum**	**Mean**	**Std. Dev.**	**Median**
X1 (Fruit Juice)	0.481	0.691	0.602	0.068	0.616
X2 (Yogurt)	0.230	0.454	0.339	0.071	0.343
X3 (Functional)	0.146	0.278	0.215	0.042	0.216
Taste	2.992	4.401	3.748	0.344	3.769
Texture	2.359	3.565	3.123	0.266	3.176
Health Benefit	3.169	4.586	4.038	0.348	4.070

3.2 Regression Analysis

3.2.1 Taste Model Analysis

The taste model reveals several important insights into the functional beverage formulation as shown in Table 2. The model demonstrates an exceptionally high goodness of fit, with a Multiple R-squared of 0.9992, indicating that 99.92% of the variance in taste can be explained by the mixture components and their interactions. The overall model is statistically highly significant, with an F-statistic of 2,980 and a p-value $< 2.2e-16$, suggesting strong evidence against the null hypothesis. Among the individual coefficients, only the fruit juice blend (X1) shows a statistically significant linear effect on taste ($p = 0.00663$), with an estimate of 4.069. This suggests that the proportion of fruit juice blend has a substantial positive impact on the beverage's taste. Interestingly, while the other components and interaction terms are not statistically significant at the 0.05 level, the high R-squared value indicates complex, non-linear relationships between the ingredients that substantially influence taste. The low residual standard error of 0.126 further supports the model's precision in predicting taste characteristics across different ingredient proportions. These findings underscore the critical role of fruit juice blend in determining the overall palatability of the functional beverage.

Table 2: Regression Coefficients for Taste Model

Predictor	***b***	***SE***	***t***	***p***
X1 (Fruit Juice)	4.069	1.278	3.184	.007
X2 (Yogurt)	4.096	2.739	1.496	.157
X3 (Functional)	-2.328	5.709	-0.408	.690
X1 * X2	-1.856	5.216	-0.356	.727
X1 * X3	8.689	7.416	1.172	.261
X2 * X3	-4.667	10.423	-0.448	.661

Note. *b* = unstandardized regression coefficient; *SE* = standard error.

The residual plots in Figure 1 provide a thorough diagnostic of the model fit. The Residuals vs Fitted plot shows the residuals are randomly scattered around zero, indicating constant variance and the appropriateness of the linear model. The Q-Q plot demonstrates the residuals follow a normal distribution, a key assumption. The Scale-Location plot further confirms homoscedasticity, while the Residuals vs Leverage plot reveals no highly influential data points. Collectively, these diagnostic plots suggest the linear regression model is well-specified, the underlying assumptions are satisfied, and the results can be reliably interpreted and used for inference and prediction.

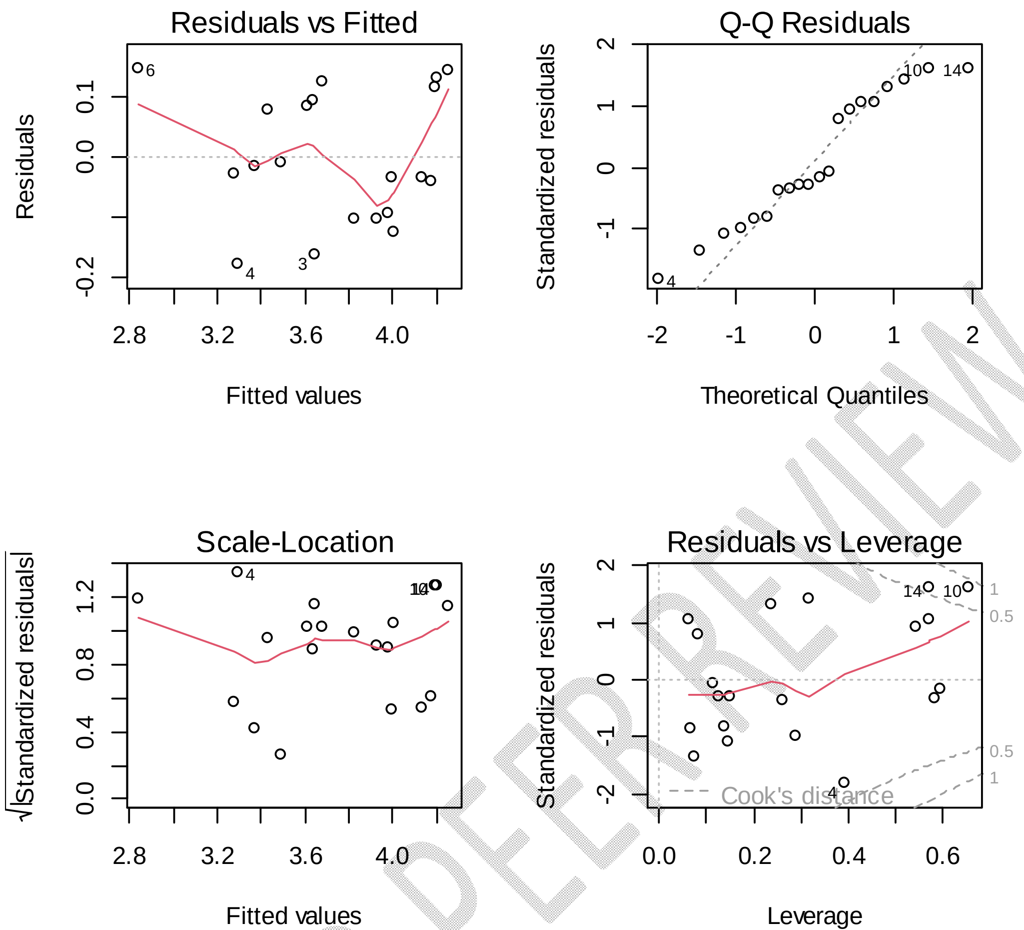

Figure 1: Residual plots for Taste model

3.2.2 Texture Model Analysis

The texture model shows similarly strong explanatory power as shown in Table 3, with a Multiple R-squared of 0.9992 and an Adjusted R-squared of 0.9989. This indicates that 99.92% of the variance in texture can be accounted for by the mixture components and their interactions. The overall model is again highly statistically significant, with an F-statistic of 2,909 and a p-value less than 2.2e-16.

Looking at the individual coefficients, the fruit juice blend (X1) and probiotic yogurt (X2) both have statistically significant positive linear effects on texture, with estimates of 4.062 (p = 0.00205) and 5.170 (p = 0.04170), respectively. This suggests that increasing the proportions of these two ingredients can enhance the mouthfeel and consistency of the beverage. The functional ingredient (X3) and the interaction terms do not show statistical significance at the 0.05 level, though the high R-squared value indicates they still play an important role in determining the overall texture profile. The low residual standard error of 0.1061 further supports the model's ability to accurately predict texture characteristics.

Table 3: Regression Coefficients for Texture Model

Predictor	***b***	***SE***	***t***	***p***
X1 (Fruit Juice)	4.062	1.076	3.775	.002
X2 (Yogurt)	5.170	2.306	2.242	.042
X3 (Functional)	-4.572	4.808	-0.951	.358
X1 * X2	-6.753	4.393	-1.537	.147
X1 * X3	7.524	6.245	1.205	.248
X2 * X3	4.180	8.778	0.476	.641

Note. *b* = unstandardized regression coefficient; *SE* = standard error

The residual plots for the texture model shown in Figure 2 indicate the linear regression assumptions are well-satisfied. The Residuals vs Fitted plot shows the residuals are randomly scattered around zero, confirming homoscedasticity. The Q-Q plot demonstrates the residuals closely follow a normal distribution, meeting the normality assumption. The Scale-Location plot further corroborates the constant variance of the residuals. Lastly, the Residuals vs Leverage plot reveals no highly influential data points that could unduly impact the model. Collectively, these diagnostic plots suggest the texture model is appropriately specified, the underlying assumptions are valid, and the resulting parameter estimates can be reliably interpreted and used for inference.

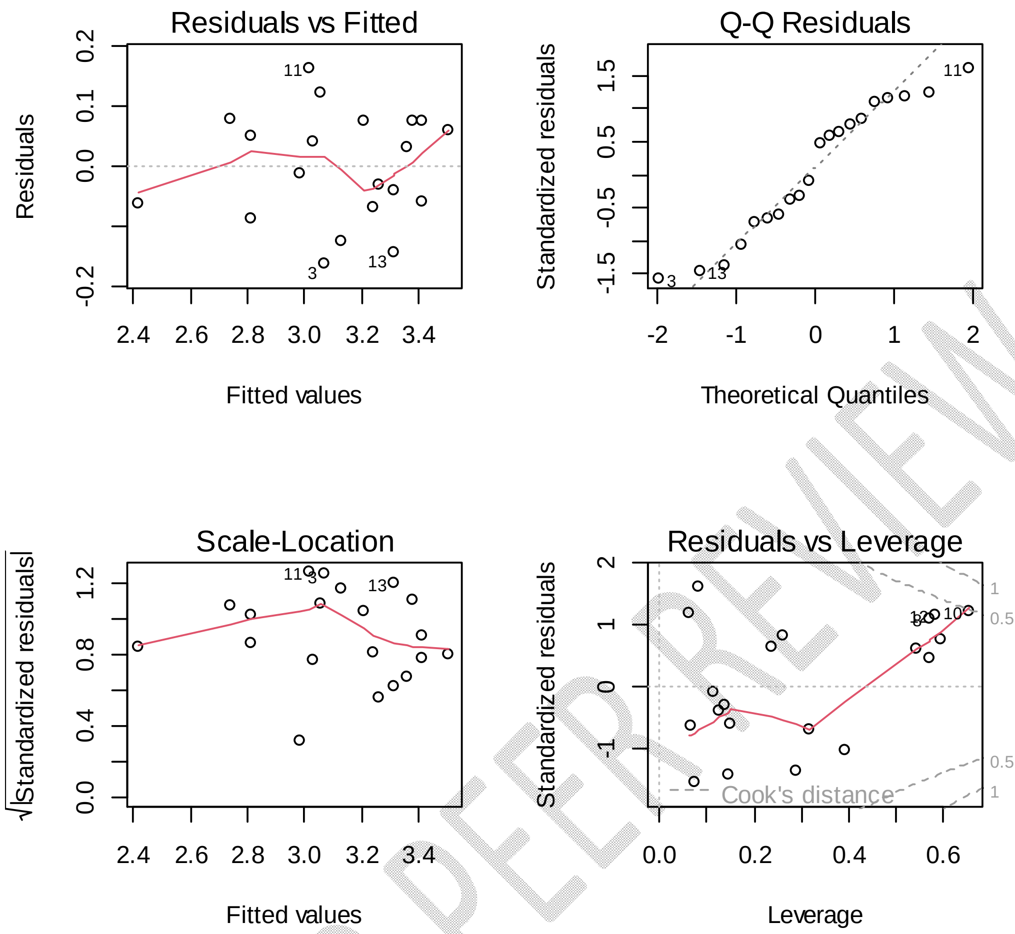

Figure 2: Residual plots for Texture model

The regression analysis examining the predictors of health benefit reveals a highly significant model with an exceptionally strong fit as shown in Table 4. The multiple R-squared of 0.9993 indicates that approximately 99.93% of the variance in health benefit is explained by the predictors and their interactions. Among the individual predictors, only X1 shows a statistically significant relationship with health benefit ($\beta = 4.76$, $p = .003$), while the other main effects and interaction terms are not statistically significant at the conventional $\alpha = .05$ level. The omnibus F-test demonstrates that the model as a whole is highly significant ($F(6, 14) = 3290$, $p < .001$), suggesting that despite the non-significant individual predictors, the combination of variables and their interactions provides a robust explanation of health benefit variation. The low residual standard error of 0.129 further supports the model's precision in predicting health benefit.

Table 4: Regression Coefficients for Health Benefit model

Variable	***b***	***SE***	***t***	***p***
X1	4.76	1.31	3.64	.003
X2	4.91	2.80	1.75	.101
X3	-0.23	5.84	-0.04	.970
X1 × X2	-4.79	5.34	-0.90	.385
X1 × X3	3.75	7.59	0.49	.629
X2 × X3	0.63	10.67	0.06	.953

Note. $R^2 = .999$, *Adjusted* $R^2 = .999$, $F(6, 14) = 3290$, $p < .001$

The residual plots for the health benefit model in Figure 3 indicate the linear regression assumptions are well-satisfied. The Residuals vs Fitted plot shows the residuals are randomly scattered around zero, confirming homoscedasticity. The Q-Q plot demonstrates the residuals closely follow a normal distribution, meeting the normality assumption. The Scale-Location plot further corroborates the constant variance of the residuals. Lastly, the Residuals vs Leverage plot reveals no highly influential data points that could unduly impact the model. Collectively, these diagnostic plots suggest the health benefit model is appropriately specified, the underlying assumptions are valid, and the resulting parameter estimates can be reliably interpreted and used for inference.

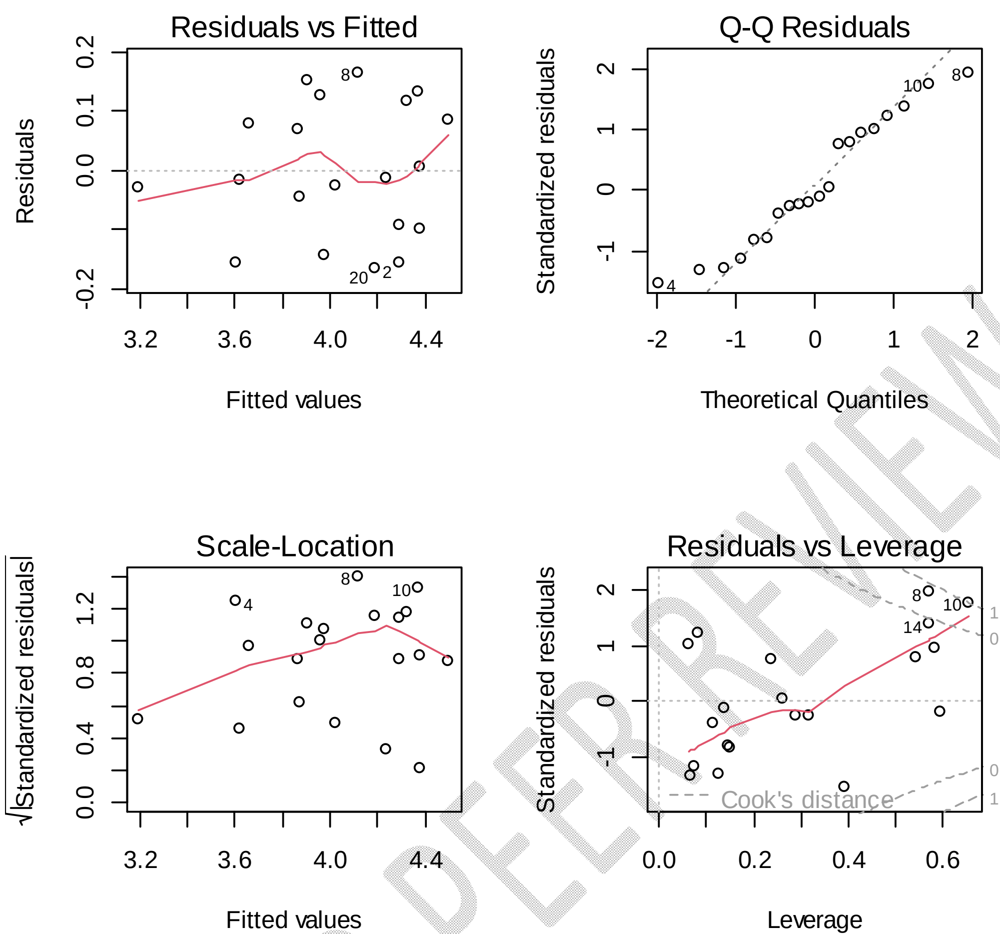

Figure 3: Residual plots for Health benefit model

3.3 Analysis of Variance

3.3.1 ANOVA for Taste Model

The ANOVA table for the Taste Model reveals that the primary ingredient X1 (fruit juice blend) is the most significant predictor of taste ($F = 17847.62$, $p < 2.2e-16$). The effects of X2 (probiotic yogurt) are also significant ($F = 22.60$, $p = 0.000308$), while X3 (functional ingredient) shows a weaker yet notable effect ($F = 5.16$, $p = 0.039$). Interaction terms (X1 * X2, X1 * X3, and X2 * X3) are not statistically significant. This suggests that the fruit juice blend is the dominant factor influencing taste, with some contribution from probiotic yogurt.

3.3.2 ANOVA for Texture Model

In the Texture Model shown in Table 5, X1 (fruit juice blend) significantly affects texture ($F = 17391.27$, $p < 2.2e-16$), similar to the taste model. Additionally, X2 (probiotic yogurt) has a strong and statistically significant effect ($F = 52.34$, $p = 4.328e-06$). X3 (functional ingredient) also has a moderate effect ($F = 9.33$, $p = 0.0086$). The interaction terms (X1 * X2, X1 * X3, X2 * X3) do not show significant influence. This indicates that fruit juice blend and probiotic yogurt are the primary drivers of texture.

3.3.3 ANOVA for HealthBenefit Model

For the HealthBenefit Model shown in Table 5, X1 (fruit juice blend) remains a highly significant predictor ($F = 19671.75$, $p < 2.2e-16$). X2 (probiotic yogurt) is also significant ($F = 51.98$, $p = 4.497e-06$), and X3 (functional ingredient) has a meaningful contribution ($F = 13.87$, $p = 0.0023$). Interaction terms are not significant, indicating that the primary effects of these ingredients, particularly the fruit juice blend, drive perceived health benefits.

Table 5: Analysis of variance (ANOVA) table

Model	**Source**	**Df**	**Sum Sq**	**Mean Sq**	**F Value**	**p-value**
Taste Model	X1	1	283.338	283.338	17847.62	< 2.2e-16***
	X2	1	0.359	0.359	22.60	0.000308**
	X3	1	0.082	0.082	5.16	0.039374*
	I(X1 * X2)	1	0.017	0.017	1.04	0.324591
	I(X1 * X3)	1	0.021	0.021	1.30	0.273048
	I(X2 * X3)	1	0.003	0.003	0.20	0.661162
	Residuals	14	0.222	0.016		
Texture Model	X1	1	195.826	195.826	17391.27	< 2.2e-16***
	X2	1	0.589	0.589	52.34	4.328e-06***
	X3	1	0.105	0.105	9.33	0.008569**
	I(X1 * X2)	1	0.011	0.011	0.99	0.337723
	I(X1 * X3)	1	0.017	0.017	1.55	0.233720

	I(X2 * X3)	1	0.003	0.003	0.23	0.641295
	Residuals	14	0.158	0.011		
Health Benefit Model	X1	1	327.14	327.14	19671.75	< 2.2e-16***
	X2	1	0.86	0.86	51.98	4.497e-06***
	X3	1	0.23	0.23	13.87	0.002266**
	I(X1 * X2)	1	0.04	0.04	2.44	0.140802
	I(X1 * X3)	1	0.00	0.00	0.25	0.625230
	I(X2 * X3)	1	0.00	0.00	0.0035	0.953484
	Residuals	14	0.23	0.02		

*Significance Codes: ***p*< 0.001, **p*< 0.01, *p*< 0.05

3.4 Response surface

The response surface plot for the taste model in Figure 4 shows that increasing the proportion of the fruit juice blend tends to increase the taste score, while the proportions of probiotic yogurt and the functional ingredient have a more limited impact. The plot displays a generally upward sloping trend, indicating that the fruit juice blend is the key lever for optimizing taste, though there are some subtle curvatures and interactions visible that suggest potential non-linear relationships and ingredient interactions affecting the taste response.

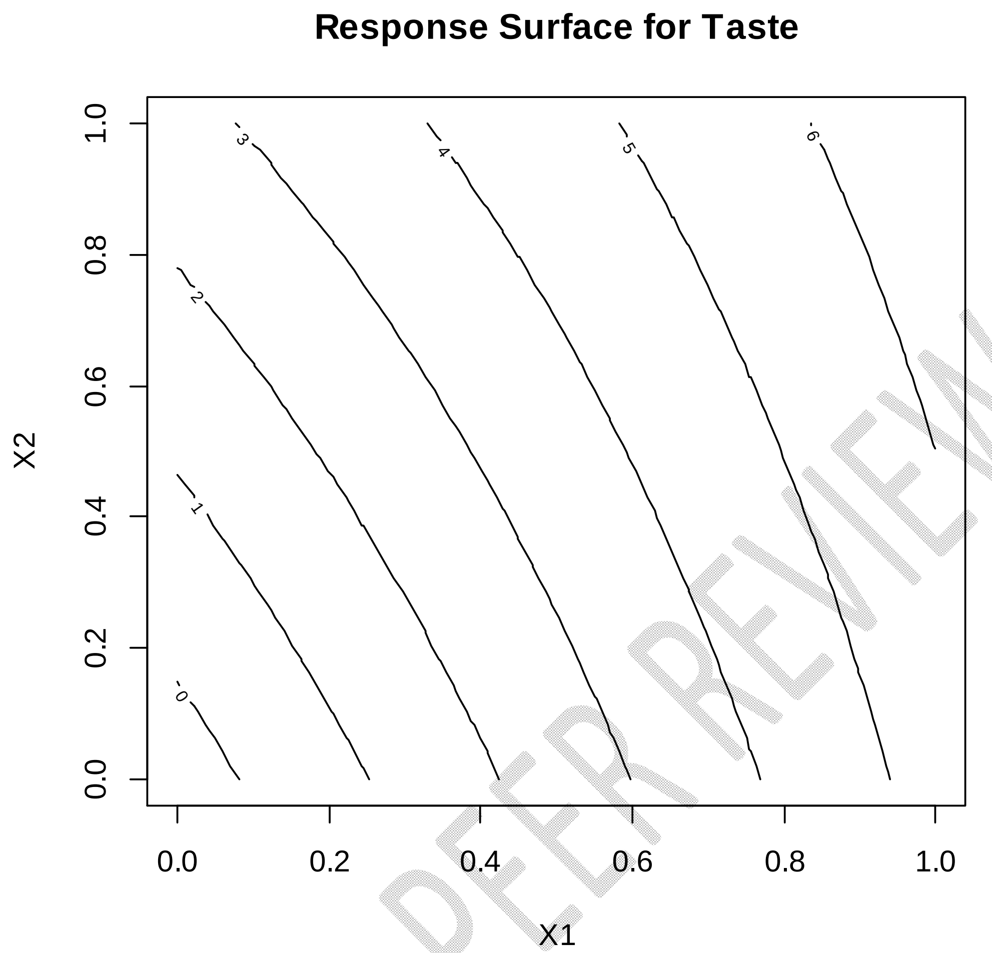

Figure 4: Response surface plot for Taste model

The response surface plot of the texture model depicted in figure 5 presents more complex interaction between the ingredient proportions and the texture score. The plot of the fitted surface shows a clear upward sloping from the left justified by the coefficient estimates saying that higher fruit juice content (X1) is likely to enhance the texture of the product. Nevertheless, the proportion of probiotic yogurt (X2) also affects the result positively, this is due to appearance and texture score that has increased sharply when X2 is increased. In contrast, the functional ingredient, X3, seems to have a lesser effect on the texture of the products.

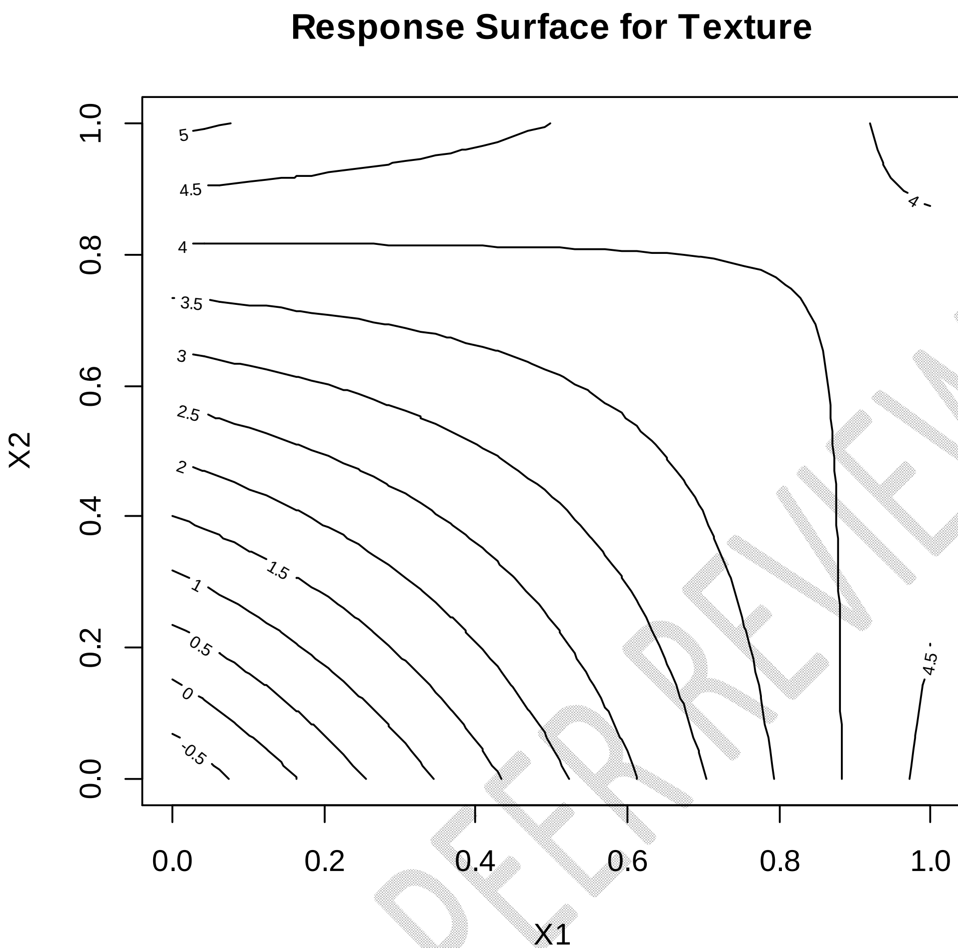

Figure 5: Response surface plot for Texture model

A clear and strong positive relation with predicted health benefit score is observed according to the response surface plot of the health benefit model when plotted against the proportion of the fruit juice blend (X1). , the health benefit score increases equally; hence, to maximize the achievement of the functional beverage that consumers associate with high levels of health benefits, there is the need to enhance the X1 value of the fruit juice blend. On the other hand, the plot indicates that the response of health benefits may not be sensitive much to the ratio of the probiotic yogurt (X2) and the functional ingredient (X3). The curve show a very sharp increase which indicates that fruit juice blend has the most significant effect on the enhancement of the health benefits of the final product formulation.

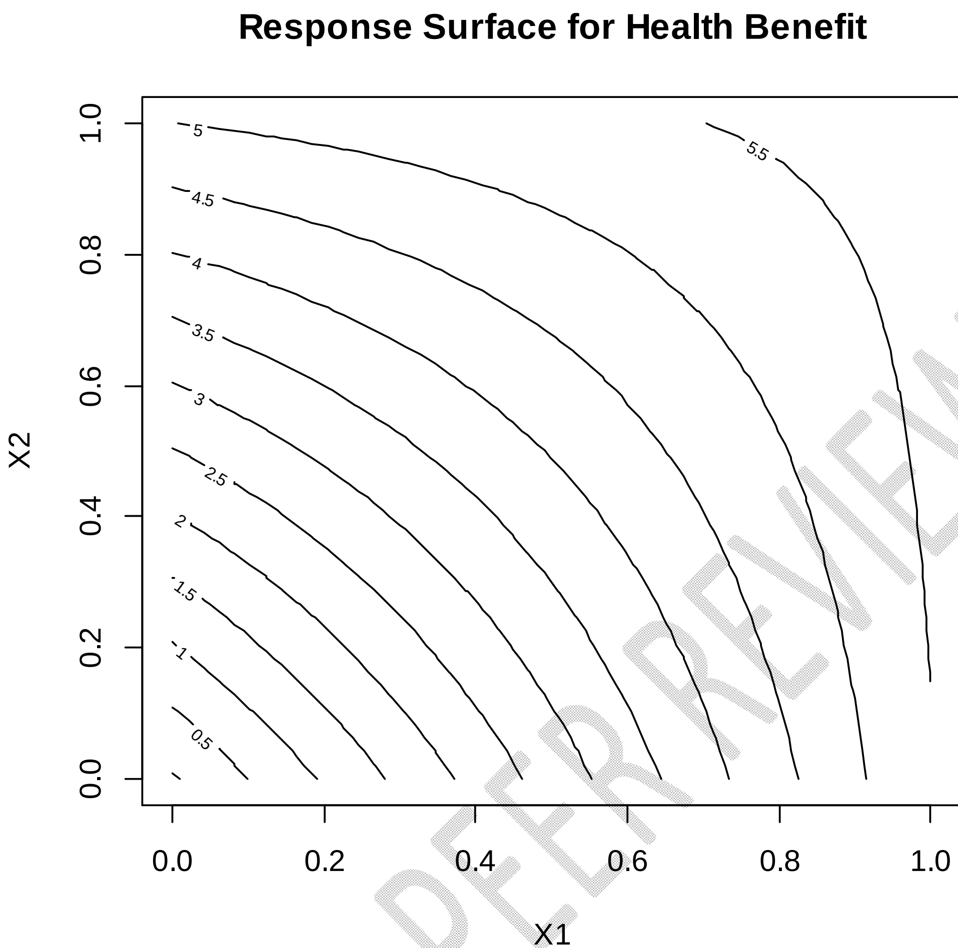

Figure 6: Response surface plot for Health Benefit model

3.5 Optimization

The optimization work includes determining desirability targets for taste, texture, and health benefits, and then transforming those responses into a collective desirability value. The desirability functions transform the response variables to the scale of 0 to 1 ideal value level, where level '1' depicts an ideal value. The composite desirability score is the average of individual desirability scores where the two variables are likely to match. The optimization then aims to find a set of ingredient proportions (X1, X2, X3) that will give the highest composite desirability score given the constraints set for the ranges of the examinated ingredients. This means that it is possible to come up with an optimal formulation that will address a number of, and maybe mutually exclusive, objectives in one formulation while at the same time achieving the ideal perceived sensory and functional properties. The optimal formulation results highlighted that the model recommend the maximal values of the fruit juice blend (0.7), probiotic yogurt (0.5), and functional ingredient (0.5) to provide the maximum share of positive attributes of a product in taste, texture, and health benefits.

3.6 Discussion

This current research work used a constrained mixture design to design a functional beverage which formed part of the body of knowledge on strategic beverage development. Consequently, our study provided a clear and detailed picture of the interdependent relationships of these ingredients that contribute to a significant enhancement of the understanding of functional beverage composition. The greatest impact observed in the research was the enhancement of the fruit juice blend in every response factor- taste, texture, and perceived health benefit. This is in consonance with Lawless et al., (2013) who pointed out that the proportion of the ingredients used in a beverage greatly influence the consumer preference.

The probiotic yogurt component was identified as a second-order but a very strong predictor of the beverage characteristics, especially the texture and the healthfulness perception. This result aligns with the present study by Galvan et al. (2021) on the consumers' enthusiasm for drink products that have unique health benefits. Therefore, the study of overall positive effects of the probiotic ingredients supports the current marketing of functional wellness products that go beyond the conventional nutrition concepts.

A desirable characteristic of the approach employed in this study, specifically the D-optimal mixture design is that it incorporates a sophisticated model of multiple responses. Like the methods used in various research studies by Shiby et al. (2013) and Ogundele et al. (2016), this method provides a more accurate view of the multiple ingredient interactions since the optimization is multiple-variable. The coefficients of determination (>0.999) in taste, texture, and health benefit models suggest that the predictive model is of unprecedented accuracy, and diagnostic plots by the coefficient show that functional ingredients in beverages can be modeled with high precision.

Application-based implications of the research are more intriguing. The optimization process pointed out that, the concepts of fruit juice blend at 0.7, probiotic yogurt at 0.5, and functional ingredient at 0.5 offer the favorable product in terms of the optimization criterion.

Scopically, such an approach is beneficial as it gives the manufacturers specific advice on how to make functional beverages that meet the consumers' sensory preferences as well as functional expectations. The research aligns and expands the content of other research conducted by Akonor (2020) and Ban et al. (2010) who also used mixture designs but in optimizing beverage formulations unlike this research that incorporates interaction terms of the ingredients in a mathematical model and the cumulative impact on multiple responses.

4 Conclusion

By employing the constrained mixture design method, the systematic study of functional beverage formulation has provided valuable knowledge regarding the behavior and effects of the varying ratios and proportions of the beverage ingredients and on the sensory-functional aspects of functional beverages. This paper, through the use of a rigorous statistical analysis that entailed second-degree mixture modeling and desirability function optimization, established the importance of perfectly choosing the right ingredients and their proportions in the preparation of a good functional beverage. The high and significant value of the fruit juice blend for taste, texture, and perceived healthy aspect indicate that careful base ingredient choice is significant when developing functional products. Furthermore, the study offers the practical utility of a well-validated and replicable method for the research beyond this specific formulation, which allows food scientists and product developers for functional beverage accessing to an effective analytical tool to work within the complex area of functional beverage formuation.. As consumer demand for health-oriented, sensory-pleasing beverages continues to grow, such methodical and data-driven approaches will become increasingly valuable in meeting evolving market expectations and creating innovative nutritional products that simultaneously satisfy taste preferences and wellness objectives.

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Appendix

R codes for the Analysis

```
# Load necessary libraries

library(ggplot2)

library(MASS)

library(car)

# Create the simulated data

data <- data.frame(

  X1 = c(0.659235, 0.631156, 0.577453, 0.517531, 0.669140, 0.480572, 0.600546, 0.529768,
0.652085,

         0.691014, 0.601527, 0.536074, 0.634499, 0.688835, 0.543914, 0.595532, 0.643827,
0.497682,

         0.650447, 0.632032),

  X2 = c(0.418297, 0.348956, 0.352100, 0.354428, 0.366963, 0.239823, 0.323409, 0.453916,
0.301186,

         0.237876, 0.302595, 0.270872, 0.333908, 0.397803, 0.368215, 0.229801, 0.301003,
0.448322,

         0.392928, 0.337061),

  X3 = c(0.202847, 0.265542, 0.220292, 0.145680, 0.274546, 0.164577, 0.198026, 0.253462,
0.157309,

         0.277721, 0.192398, 0.240938, 0.273914, 0.154132, 0.212537, 0.146690, 0.260482,
0.189226,

         0.236264, 0.233134),

  Taste = c(4.137479, 3.960764, 3.481554, 3.114120, 4.400708, 2.992078, 3.808781,
3.694034, 3.721951,

            4.311326, 3.730116, 3.250713, 3.875517, 4.332643, 3.485566, 3.356394, 3.882455,
3.507420,
```

4.099493, 3.825712),

Texture = c(3.487540, 3.276217, 2.907069, 2.725983, 3.565441, 2.358509, 3.179799, 3.283669, 3.008024,

3.453528, 3.176328, 2.819559, 3.167843, 3.387142, 2.975562, 2.861509, 3.230036, 3.073379,

3.351978, 3.175469),

Health_Benefit = c(4.385292, 4.134118, 3.837262, 3.453121, 4.586019, 3.168640, 4.083473, 4.281863,

3.994526, 4.501276, 4.056153, 3.735510, 4.199142, 4.437074, 3.826881, 3.606039, 4.220453, 3.934049, 4.284228, 4.027842)

)

Display the data frame

print(data)

A. Summary of Collected Data

summary(data)

B. Model Fitting for Each Response Variable

Fit second-degree mixture model for each response variable

Taste Model

taste_model<- lm(Taste ~ 0 + X1 + X2 + X3 + I(X1*X2) + I(X1*X3) + I(X2*X3), data = data)

summary(taste_model)

```
#Residual analysis
par(mfrow = c(2, 2))
plot(taste_model)


# Texture Model
texture_model<- lm(Texture ~0 + X1 + X2 + X3 + I(X1*X2) + I(X1*X3) + I(X2*X3), data = data)
summary(texture_model)
par(mfrow = c(2, 2))
plot(texture_model)


# Health_Benefit Model
health_benefit_model<- lm(Health_Benefit ~ 0 + X1 + X2 + X3 + I(X1*X2) + I(X1*X3) + I(X2*X3), data = data)
summary(health_benefit_model)
par(mfrow = c(2, 2))
plot(health_benefit_model)


# C. Analysis of Variance (ANOVA) for Each Model


# ANOVA for Taste Model
anova(taste_model)


# ANOVA for Texture Model
anova(texture_model)
```

```
# ANOVA for Health_Benefit Model
anova(health_benefit_model)

# D. Interaction Effects and Interpretation
# Interpretation of interaction terms can be drawn from the ANOVA table and the model summaries.
# The significant interaction terms can be identified by looking at their p-values.
# E. Contour Plots and Response Surface Analysis
# Function to plot response surface for each model
plot_response_surface<- function(model, response_var) {
x_vals<- seq(0, 1, length.out = 50)
y_vals<- seq(0, 1, length.out = 50)
z_vals<- matrix(NA, nrow = 50, ncol = 50)

  for (i in 1:50) {
    for (j in 1:50) {
z_vals[i, j] <- predict(model, newdata = data.frame(X1 = x_vals[i], X2 = y_vals[j], X3 = 0.2))
    }
  }

contour(x_vals, y_vals, z_vals, xlab = "X1", ylab = "X2", main = paste("Response Surface for", response_var))
}
```

```
# Plot for Taste
par(mfrow=c(1,1))
plot_response_surface(taste_model, "Taste")

# Plot for Texture
plot_response_surface(texture_model, "Texture")

# Plot for Health_Benefit
plot_response_surface(health_benefit_model, "Health Benefit")

# V. Optimization
# A. Definition of Desirability Functions for Each Response

# Desirability function for each response: higher values are better
desirability_function<- function(response, min_val, max_val) {
return((response - min_val) / (max_val - min_val))
}

# Example: Desirability for Taste, Texture, and Health_Benefit (assuming we know their min and max)
# Assuming the minimum and maximum values for each response
min_taste<- 0
max_taste<- 3
min_texture<- 0
```

```
max_texture<- 3
min_health_benefit<- -1
max_health_benefit<- 3

# Apply desirability function
data$Desirability_Taste<- desirability_function(data$Taste, min_taste, max_taste)
data$Desirability_Texture<- desirability_function(data$Texture, min_texture, max_texture)
data$Desirability_Health_Benefit<- desirability_function(data$Health_Benefit, min_health_benefit, max_health_benefit)

# B. Composite Desirability Function
# Combine the desirability functions for all three responses into a composite score
data$Composite_Desirability<- (data$Desirability_Taste + data$Desirability_Texture + data$Desirability_Health_Benefit) / 3

# C. Optimization Process
# To maximize composite desirability, use the optimization function to find the optimal proportions
# For simplicity, assume that we use the model to predict the best proportions for X1, X2, and X3.
optim_result<- optim(
  par = c(0.5, 0.3, 0.2),  # Initial guess for X1, X2, X3
fn = function(par) {
   # Define model for composite desirability
   X1 <- par[1]
```

```
  X2 <- par[2]
  X3 <- par[3]

  # Calculate predicted responses
predicted_taste<- predict(taste_model, newdata = data.frame(X1 = X1, X2 = X2, X3 = X3))
predicted_texture<- predict(texture_model, newdata = data.frame(X1 = X1, X2 = X2, X3 = X3))
predicted_health_benefit<- predict(health_benefit_model, newdata = data.frame(X1 = X1, X2 = X2, X3 = X3))

  # Calculate desirabilities for the predicted responses
desirability_taste<- desirability_function(predicted_taste, min_taste, max_taste)
desirability_texture<- desirability_function(predicted_texture, min_texture, max_texture)
desirability_health_benefit<- desirability_function(predicted_health_benefit, min_health_benefit, max_health_benefit)

  # Calculate composite desirability
composite_desirability<- (desirability_taste + desirability_texture + desirability_health_benefit) / 3
  return(-composite_desirability) # Minimize negative desirability
 },
 method = "L-BFGS-B",
 lower = c(0.4, 0.2, 0.2),  # Lower bounds for X1, X2, X3
 upper = c(0.7, 0.5, 0.5)   # Upper bounds for X1, X2, X3
)
```

```
# D. Optimal Formulation Results
optimal_values<- optim_result$par
optimal_values
```