Optimization and Modeling of Energy Bars Based Formulations by Simplex Lattice Mixture Design

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Abstract— Simplex lattice mixture design was utilized to optimize high caloric and acceptable energy bars. Fourteen formulations of energy bars were produced from flour blends of high quality cassava flour (0-100%), toasted bambara groundnut (0-100%) and roasted cashew kernel(0-100%). The study was carried out to evaluate the effect of varying the proportions of the independent variables on these dependent variables (proteins, fats, carbohydrate) and general acceptability qualities of the energy bars. Proteins, Fats and Carbohydrates were indicators of the calorie values of these energy bars. Mixture response surface methodology was used to model the proteins, fats, carbohydrates and general acceptability with single, binary and ternary combinations of high quality cassava flour, toasted bambara groundnut and roasted cashew kernel flours. The effect of variation in levels of cassava, bambara groundnut and cashew kernel flours on the fats, proteins, carbohydrates and general acceptability of the formulated energy bars were adequately predicted with regression equation. The statistical adequacy of the generated polynomial equations of the responses were checked using the following indices: F-value at p < 0.05, coefficient of determination R^2 , Adj. R^2 , lack of fit, and coefficient of variation (CV). Optimization suggested energy bars containing 61.40 % high quality cassava flour, 0.00 % bambara groundnut flour and 38.6 % cashew kernel flour as the best proportion of these components with a desirability of 0.775. Numerical optimization indicated that better sensory and high calorific qualities are directly related with the proportion of cassava flour, bambara groundnut flour and cashew kernel flour respectively. The optimum blends as validated showed a close relationship between the predicted and experimental values.

Keywords— Optimization, proteins, fats, carbohydrates, cassava, bambara groundnut, cashew kernel.

I. INTRODUCTION

Consumers' demand and desire healthy foods that is portable, convenient and proportioned as well. Often, many options are not available that are minimally processed, rich in nutrients and tastes good (Mridula et al., 2013). The food bars are snacks of good sensory and nutritional characteristics due to their high carbohydrates, proteins, lipids and minerals contents (Ooamah, 2001). To provide consumers with ready to eat healthy foods is one of major challenges food processors encounter. Energy bars, a food product that fits these criteria, continue to increase in sales according to the AC Nielsen Market Track (BIS, 1971). The energy bars consists of flour blend (cassava, bambara groundnut and cashew kernel), date syrup, soy isolate, vegetable fats, baking soda, carboxy methyl cellulose, salt and chocolate. Bambara groundnut flour, cashew kernel flour and soy isolate are the major sources of proteins and energy. Date fruit is consumed as

fresh date or processed to different products like date syrup (DS). DS is produced commercially by extraction and concentration under vacuum the yield could be improved by using pectinase/cellulase enzymes (Al-Hooti *et al.*, 2002). DS contains 68-80% simple sugars (glucose and fructose) and other nutrients (proteins, lipids, pectin and minerals) and its quality varies depending on type of date variety used (Mostafazadeha *et al.*, 2011).

Cassava (*Manihot esculenta Crantz*) is the chief source of dietary food energy for the majority of the people living in the lowland tropics, and much of the sub-humid tropics of West and Central Africa (Tsegiaand Kormawa, 2002). Bambara is grown extensively in Nigeria but it is one of the lesser utilized legumes in Nigeria (Olapade and Adetuyi, 2007). Nigeria is one of the main producers of cashew fruit (Honorato *et al.*, 2007) but lack the industrial utilization of this wonderful cash crop.

Different food science researchers and nutritionists have documented the effectiveness of response surface methodology (RSM) in optimization of ingredient levels, formulations and processing conditions in food recipes and formulations (Cherieet al., 2018). The main advantage of RSM is the reduced number of experimental runs needed to provide sufficient information for statistically acceptable result (Giovanni, 1983). It is a faster and less expensive method for gathering research result than the classical method. RSM has successfully been applied for the development and optimization of the cereal products (Singh et al., 2004; Chakraborty et al., 2011). It is a statistical mathematical method that uses quantitative data in an experimental designto determine and simultaneously solve multivariate equations to optimize processes and products (Cox, 1971). RSM is also a useful tool to minimize the numbers of trials and provide multiple regression approach to achieve optimization (Seth and Rajamanickam, 2012). Itis a special response surface experiment in which the design factors are the components or ingredients of amixture, and the response depends on the proportions of the ingredients that are present (Myers et al., 2009). Anuar et al. (2013) and Gupta et al. (2014) suggested that numerical optimization require that goals (i.e. None, Maximum, Minimum, Target or Range) should be set for the variables and response where all goals are combined into one desirable function. In this study, good sets of conditions that will meet all the goals, the independent variables (i) cassava flour, (ii) bambara groundnut flour and (iii) cashew kernel flour were all set within range, protein, carbohydrates, general acceptability scores were set at maximum while fats was set within range.

Thus, this study was conducted to develop and optimize energy bars madefrom flour composites of high quality cassava flour, toasted bambara groundnut flour and cashew kernel flourwhich hashigh caloric value and acceptable with regard to the general acceptabilityusing mixture response surface methodology. The finding of the study will provide a guide for future commercial energy bars companies and household makers to produce a high caloric and acceptable quality energy bars with available raw material, which in turn be cost effective.

II. MATERIALS AND METHODS

2.1. Sample collection and preparation

TMS 30572 variety of cassava was obtained from the National Root Crop Institute (NRCRI) Umudike,

Abiastate. The bambara groundnut (cream brown eye) seed used was purchased from Ose market, Onitsha Anambra state while the raw cashew nuts were purchased from 'owum' in Enugu state. Cassava tubers were processed using the high grade processing method for cassava flours as described by Oti and Ukpabi (2006).

Healthy cleaned bambara groundnut seeds (4kg) was soaked in water in the ratio of 1:3 i.e one portion of bambara groundnut seed to three portion of water for 9 h. They were steamed for 20 min, cooled and dehulled. After dehulling, the cotyledons were toasted using Master chef electric toaster oven (120 °C for 1h 20 min). The toasted cotyledons were cooled and milled using milling machine. Cashew nut flour was processed using the method described by Okafor and Ugwu,(2014). The milled flour samples were sieved with a sieve of aperture size of 75 μ m screen opening to obtain the fine flour sample which was packaged properly in air tight containers.

2.2. Simplex lattice mixture design

The augmented design (Table 1) was used to replicate vertices and binary blends at the edges to minimize residual errors.

Table.1: Mixture Components Studied in Energy bar
Experiment

Low	Component	Description	High
0	A(xi)	Cassava flour	100
0	B(x2)	Bambara groundnut flour	100
0	C(x3)	Cashew kernel flour	100

Design- Expert [®], version 11.0 software was used for the generation of test formulations and analysisof the results. Augmented Simplex lattice design method was employed, to formulate recipes, study the maineffect of parameters, create models between the variables, and determine the effect of these variablesto optimize the levels of ingredients. Fourteen treatments in random order are created andresponses parameters like proteins, fats, carbohydrates and general acceptability) were evaluated(Table 2). The experimental data for each response variable were fitted to the quadratic model as:

 $\gamma = \beta_1 \chi_1 + \beta_2 \chi_2 + \beta_3 \chi_3 + \beta_{12} \chi_1 \chi_2 + \beta_{13} \chi_1 \chi_3 + \beta_{23} \chi_2 \chi_3$

Where γ is the predicted response, β_i , β_j , β_k , are the coefficient of single terms, β_{ij} and β_{ijk} are the coefficient of interactive terms.

 $X_1, X_2, X_3, X_1X_2, X_1X_3, X_2X_3, X_1X_2X_3$ are the linear terms of cassava, bambara groundnut and cashew kernel and the non-linear terms of cassava.

 Table 2: Simplex lattice coded Design for Energy bar production from cassava flour, bambara groundnut flour and cashew

 kernel flour

		κεπιει μοιπ		
Blends	Component 1 A: Cassava	Component 2 B: Bambara groundnut	Component 3 C: Cashew kernel	Responses: proteins, fats, carbohydrates, general acceptability
				acceptaomty
1	0	100	0	
2	100	0	0	
3	50	0	50	
4	0	0	100	
5	100	0	0	
6	50	50	0	
7	50	50	0	
8	0	0	100	
9	0	50	50	
10	0	100	0	
11	33.3	33.3	33.3	
12	16.7	66.6	16.7	
13	66.6	16.7	16.7	
14	16.7	16.7	66.6	

2.3. Preparation of composite flour

The flour composite blends contained high quality cassava flour, toasted bambara groundnut flour and cashew kernel flour were prepared using a formula shown inTable 2. The dry material individually were blended uniformly to homogenize and then packed intightly closed clean plastic container that kept at room temperature ($25 \pm 2^{\circ}$ C) until used.

2.4. Preparation of Energy bars

Ingredients for making "energy" snack bar include flour blend (200 g), date syrup (160 mL), soy isolate (100 g), vegetable fats (80 g), baking soda (1.6 g), carboxy methyl cellulose (1.6 g), salt (1.6 g) and chocolate (3.2 g).. All the ingredients used were procured from local market (Ose market in Onitsha). Dry ingredients such as flour blend, soy isolate, carboxyl methyl cellulose, salt and chocolate flavourwere mixed together properly in a bowl. The viscous ingredients (margarine and dates syrup) were mixed in another bowl properly using cake mixer (Kenwood). The dry ingredients were added intermittently to the wet ingredients and properly kneaded together to obtain a smooth consistency. After kneading they were placed in mold bar pans (of 5cm diameter) to shape them into bars. The bars were baked at 120°C for 35 min. After kneading they were placed in mold bar pans (of 5cm diameter) to shape them into bars. The bars were baked at 120°C for 35 min. Milk chocolate was purchased from Shoprite supermarket in Onitsha. Some of the chocolate was tempered. The tempered chocolate was poured evenly into the mould (approximately 5 mm thick). The baked bar was then placed onto the chocolate and finally coated with tempered chocolate (approximately 5 mm thick).

2.5. Chemical composition

Protein and fatcontent was determined using the method as described AOAC (2012). Carbohydrate was determined by difference (Onwuka, 2005). General adaptability represents the mean score of the sensory parameters as described by Aigster *et al.*, 2011). Analyses were performed in triplicates and are expressed as percentage in dry matter (% DM).

2.6. Sensory evaluation

Energy bars prepared from the different composite flours were evaluated for its sensory acceptability and preference by using 30 consumer participants. The general acceptance is an attribute determined by a combination of sensory perception components (taste, crumb appearance, aroma, chewiness, fracturability) of the products. The nine point hedonic scale rated from 1 (extremely dislike), 5 (neither like nor dislike)to 9 (extremely like) for evaluating the degree of liking and disliking were employed.

2.7. Statistical analysis and Optimization

Numerical optimization and graphical optimization technique were employed using theDesign ExpertTM version11..0 software (State Ease Inc.) with a criterion of cassava flour, bambara groundnut flour and cashew kernel flours kept in ranges.

III. RESULTS AND DISCUSSION

The simplex lattice design for the test parameters of energy bar produced from cassava flour, bambara groundnut flour and cashew kernel flour is displayed in Table 3. Table 4 shows the coefficients estimates, adjusted regression coefficients (R^2 adj.) and the results of model significance and lack of fit for proteins, fats, carbohydrates and general acceptability for energy bars made with blends of cassava, bambara groundnut and cashew kernel.

The MRSM application on protein data showed that quadratic model was significant (p=0.0001), no lack of fit was obtained (p=0.8752) and it could explain 95.27% of all variance in the data. The following components (bambara groundnut and cashew kernel) significantly increased the protein content as seen in the equation below:

Y = 12.49 A + 19.01 B + 28.18 C $+ 11.87 \text{ AB} \quad (\text{Eqn. 1})$ Where A = cassava flour, B = bambara groundnut, C = cashew kernel

Equation (1) shows that the response value increased with increase of the variables. Among the linear component mixtures, cashew kernel flour produced the highest increase in protein values of the energy bars followed by bambara groundnut respectively. Because C > B >A, we will conclude, that component C (cashew kernel flour) produces energy bars with the highest protein content. Equation (1) revealed that increasing the linear components increased the protein content of the energy bars. The model explains 97.09 % of the variations in the protein score. Figure 1 present the contour plot of predicted protein value and a three-dimensional response surface plot. These higher response values seem to form a ridge running to the lower right of the graph. The lower left and the upper right of the graph represents mixture components that result in medium and the least protein scores respectively. The plot also showed that a blend of component A and B gave an energy bar with a protein

score of less than 20 % while mixtures of B and C gave a protein content of more than 20 %. Maximum protein score was obtained by the combination of blend B (bambara groundnut) and C (cashew kernel flour) in the contour plot. This is in close agreement with the fact that cashew kernel and bambara groundnut are good sources of protein.

The quadratic model for the fat content of the energy bars was significant (p=0.0001), interactive terms AC and BC were significant (0.0015, 0.0025) and no lack of fit was obtained (p=3.27) (Table 4.). The high R^2 and adjusted R^2 indicate a good explanation of the variability by the selected model for protein of energy bars (0.9791 and 0.9660). The regression model for predicting the fat content of the energy bars is shown in Equation (2) below:

Y = 10.38 A + 12.24 B + 34.02 C - 28.40 AC

– 26.14BC (Eqn. 2)

From the regression equation (2), linear and binary combinations of the three flour components had influence on the fat content of the energy bars. This also revealed that increasing the linear components increased the fat content of the energy bars while the binary combinations had antagonistic effects on the fat content of the energy bars. Among the linear blends, cashew kernel flour produced the highest increase in fat content followed by bambara groundnut flour and cassava flour. Among the binary blends, the blend of cassava flour and cashew kernel flour resulted in the highest antagonistic effect. High R^2 adj. (96.60 %) suggests that the effect of the independent variables contributed 96.60 % of the observed changes in the fat content of the energy bar and the adequacy of the model in predicting the fat content of the energy bars. The remaining 3.40 % changes in the fat content are because of extraneous variables not considered in the experiment. The contour plot (Figure 2) showed that the relationship between the independent variables (cassava flour, bambara groundnut flour and cashew kernel flour) and the dependent variable (response 'fats') that was used to produce the energy bars. The lower response values seem to form a ridge running to the upper left of the graph. The lower right of the graph represents mixture components that results in high fat scores respectively. Maximum fat score (27.03 %) was obtained from a blend of 87 % of component C and 13% of component B with component A set at its central value. This showed that those formulations having higher cashew kernel flour in the recipe had a relative maximum fat value which is in agreement with the fact that cashew kernel is a good sources of fats. The judicious use of cashew kernel in the diet in suitable proportions is able to enhance dietary quality with respect to fat and protein.

Analysis of variance (quadratic fit) effects of A, B, C and AC, BC interactions were significant and used in optimizing the response (carbohydrate content). No lack of fit was obtained (p=0.4113) so this can be used in predicting the carbohydrate content of energy bars. The high R^2 and adjusted R^2 indicate a good explanation of the variability by the selected model for carbohydrate content of the energy bars (0.9814 and 0.9697) (Table 4). The high R^2 and adj. R^2 indicates that the rawmaterials are good sources of carbohydrate. The model that explains the relationship between the carbohydrate content of the energy bars and the independent variables (A, B, C) is shown in Equation (4) below:

$$Y = 59.19 \text{ A} + 48.14 \text{ B} + 21.23 \text{ C} + 19.83 \text{ AC} + 30.61 \text{ BC}$$
 (Eqn. 4)

From the regression equation (4), linear and binary combinations of the three flour components had influence on the carbohydrate content of the energy bars. The linear and binary combinations increased the carbohydrate content of the energy bars. Cassavaflour (linearterm) exhibited the highest effect in increasing the carbohydrates content of the energy bars than bambara groundnutflour and cashew kernelflour by having the highest positive coefficient than the othertwoflours. Among binarycombinations, the combination of cassavaflour and cashew kernelflourexhibited the highest effect on the carbohydrate content of the energy bars followed by combination of bambara groundnutflour and cashew kernelflour. The plot showed how variable A (cassava flour) and variable B (bambara groundnut) or variable B and C (cashew kernel) affected the quality (contours) of the percentage carbohydrates. The non-linear appearance of contours curves implies strong quadratic interactions (Figure 3). In the contour plot, the lower response values seem to form a ridge running to the lower left of the graph. Maximum carbohydrate score of the energy bars (56.07 %) was obtained from a blend of 0.864 % cassava flour with 0.136% cashew kernel flour with bambara groundnut flour set at its central value. This showed that those formulations having higher cassava flour in the recipe showed relatively maximum carbohydrate value which confirms the report of El-Sharkawy (2003) that cassava is a major source of carbohydrates.

There was significant influence of the linear and quadratic terms (p=0.0001) on the general acceptability of the energy bars. The insignificant lack of fit (p=0.1015) is good even though it is non-significant. The high R^2 and adjusted R^2 indicate a good explanation of the variability by the selected model for the general acceptability of the energy bars (0.9865 and 0.9781). The model equation

obtained from the data for the general acceptability of the energy bars was:

$$Y = 6.66 \text{ A} + 5.40 \text{ B} + 7.03 \text{ C} + 1.04 \text{ AB} - 2.09 \text{ BC} \quad (\text{Eqn. 5})$$

Equation (5) suggests that the linear terms and the binary combinations contributed to the general acceptability of the energy bars. Blend BC have antagonistic blending effects .The linear terms had significant (p=0.0001) influence of the on the general acceptability of the energy bars with cashew kernel flour producing the highest increasing effect. This was followed by cassava then finally bambara groundnut flours. The model could explain 97.81 % of all variances of the hedonic results while the remaining 2.19 % could be attributed external factors not analyzed. From the contour plot (Figure 4), maximum general acceptability is obtained from a blend consisting of about 22.22 % of component A and 77.78 % component C. These higher response values seemed to form a ridge running to the extreme right of the graph. Formulations having high to medium content of bambara groundnut flour in the recipe had shown a relatively low acceptability value.

3.5. Optimum formulation

Primary objective of this study is to develop an energy bar having high qualities with regard to its protein, fats and carbohydrates values. Sensory scores for general acceptability were considered for the optimization because it was obtained from the average of all other sensory parameters. The ingredients (cassava, bambara groundnut and cashew kernel) were set in ranges. The relative importance of "3" was assigned to protein and carbohydrates. This is because the variables (protein and carbohydrates) are considered equally important in their influence on the energy content of the energy bars. Although fats plays very important role in the energy score, considering the shelf stability, the fats was minimized to a relative importance of "5" in order to ensure a shelf stable bar. The high relative importance of "5" was assigned to the general acceptability values. This is because the general acceptability represents the mean score of all the sensory parameters. Optimization suggested that energy bars made with 61.40 % cassava flour, 0.00 % bambara groundnut and 38.60 % cashew kernel flour achieved the best solution for this combination of variables with a desirability of 0.775 (Figure 5). Graphical optimization also indicated similar results (Figure 6). The predicated responses for the developed energy bar were 20.76 % proteins, 12.77 % fats, 49.42 % carbohydrates and 6.86 for general acceptability.

 Table 3: Experimental design used to develop and analyze Energy bars produced from cassava flour, bambara groundnut
 flour and cashew kernel flour

					Responses		
Blend s	Component 1 A: Cassava	Component 2 B: Bambara groundnut	Component 3 C: Cashew kernel	Proteins	Fats	Carbohydrate s	General acceptabili ty
	-					· · · · ·	
1	0	100	0	20.59	13.65	45.79	5.46
2	100	0	0	12.01	10.53	60.71	6.66
3	50	0	50	22.27	15.02	44.96	6.62
4	0	0	100	27.98	33.80	20.17	6.82
5	100	0	0	12.92	9.34	58.00	6.36
6	50	50	0	20.10	10.32	50.55	6.31
7	50	50	0	17.61	10.69	51.98	6.22
8	0	0	100	28.11	34.87	21.55	6.71
9	0	50	50	23.49	17.76	41.37	5.60
10	0	100	0	17.95	11.18	50.08	5.35
11	33.3	33.3	33.3	22.29	12.83	44.96	6.26
12	16.7	66.6	16.7	20.11	10.23	50.23	5.81
13	66.6	16.7	16.7	18.81	12.86	52.56	6.62
14	16.7	16.7	66.6	26.25	18.16	40.19	6.68

Formulation nos. 11–14 and 4 replicateruns as recommended by Design-Expert Software (11.0.3).

Table 4: Coefficient estimates, model significance, coefficient of determination (R^2) , adjusted regression coefficient (adj. R^2) and lack of fit values for the proteins, fats, carbohydrates and general acceptability of energy bars produced from high quality cassava, toasted bambara groundnut and roasted cashew kernel flours

Variables	Protein	Fats	Carbohydrates	General acceptability	
А	12.49	10.38	59.19	6.66	
В	19.01	12.24	48.14	5.40	
С	28.18	34.02	21.23	7.03	
AB	11.87	-2.51	-9.83	1.04	
AC	9.42	-28.40	19.83	0.2406	
BC	-0.4841	-26.14	30.61	-2.09	
ABC	-	-	-	-	
Model (Prob>F)	0.0001*	0.0001*	0.0001*	0.0001*	
\mathbb{R}^2	97.07	97.91	0.9814	0.9865	
Adj.R ²	0.9527	0.9660	0.9697	0.9781	
Lack of fit	0.8752n.s	3.27n.s	0.4113n.s	0.1015 n.s	

A: cassava flour; B: bambara groundnut flour; C: cashew kernel flour n.s: non-significant;*Significant at the 5% level (p<.05).

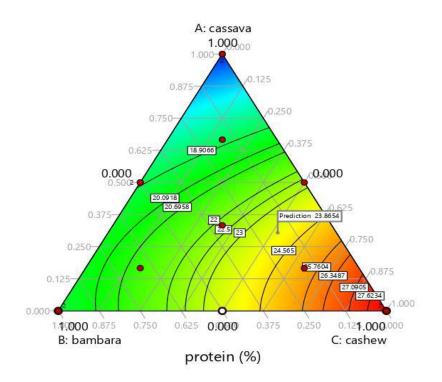


Fig.1: Contour and 3D surface plots for proteins obtained using actual-components.

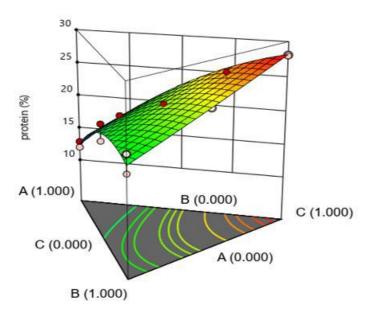


Fig.2: Contour and 3D surface plots for fats obtained using actual-components.

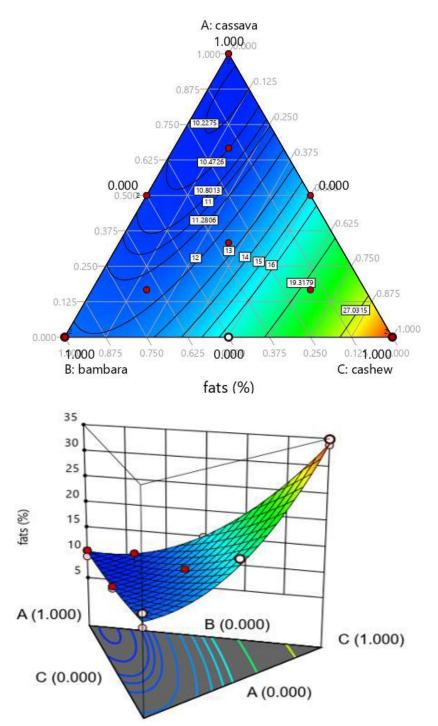


Fig.3: Contour and 3Dsurface plots for carbohydrate obtained using actual-components.

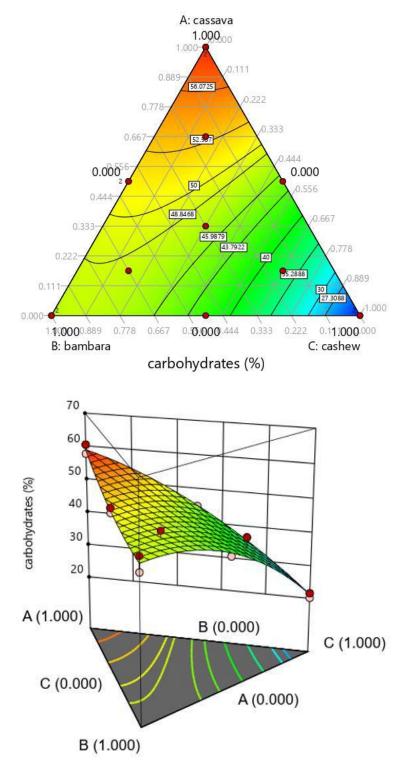


Fig.4: Contour and 3D surface plots for general acceptability obtained using actual-components.

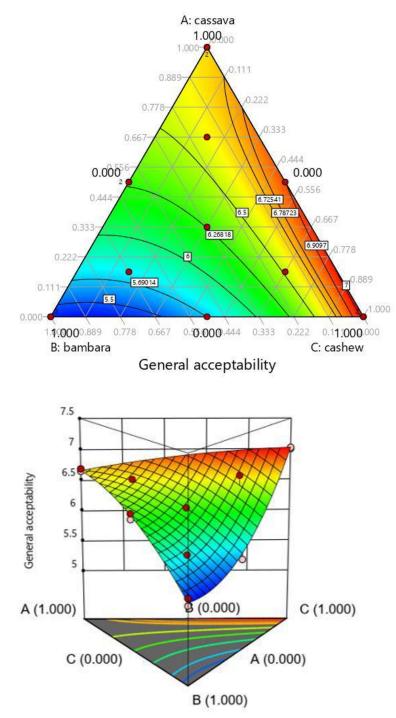


Fig.5: Contour and 3D surface plots of the desirability for multiple response function.

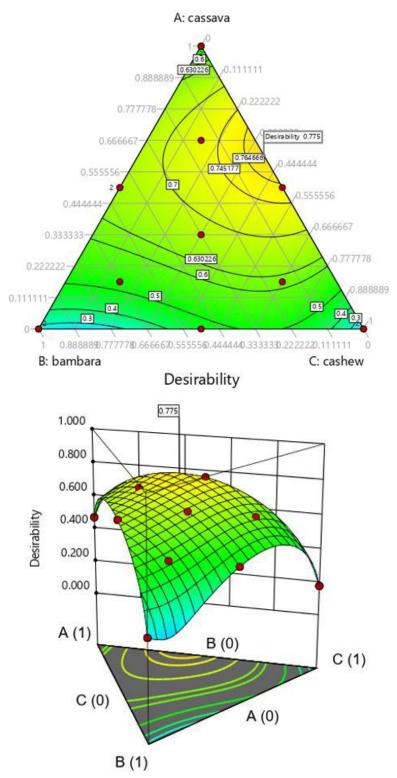
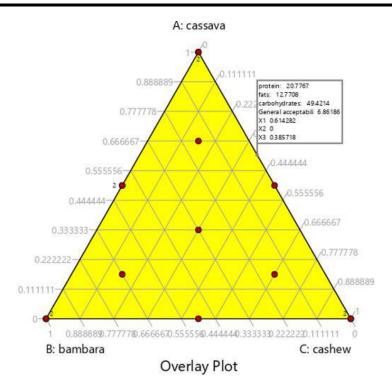


Fig.6: Contour plotsillustrating the optimum responses using graphical optimization.



IV. CONCLUSIONS

Response surface methodology was successfully applied to obtain the best combination of cassava, bambara groundnut and cashew kernel flours for producing energy bars. The optimum formula of energy barsin terms of protein,fat, carbohydrate and general acceptabilityconsisted of 61.40 % high quality cassava, 0.00% bambaragroundnut and 38.60% cashew kernel flourwith a desirability of 0.775. Theoptimized energy bar hadprotein, fat, carbohydrate and general acceptability values of 20.76 %, 12.77 %, 49.42 % and 6.86, respectively.Numerical optimization also indicated that better fats, protein and carbohydrates are directlyrelated with the proportion of cassava, bambara groundnut and cashew kernel flours, respectively. The finding of the study willprovide a guide for commercial energy bar companies and household makers to produce a high nutritional and acceptable energy bars with lower production cost.

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