ORIGINAL RESEARCH ARTICLE

Modelling and prediction of hydrolysis index of gluten-free cookies from cardaba banana starch vis-ȧ-vis response surface methodology and support vector machine.

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Abstract
The increase in the onset of celiac disease among the world populace had increased the demand for gluten-free products. Therefore, this study aimed at modelling and predicting the hydrolysis index of gluten-free cookies using response surface methodology (RSM) and support vector machine (SVM). The baking temperature (150 -180 ℃) and baking time (15-25 min) were varied using a central composite design. The obtained result revealed that both modelling approaches (RSM and SVM) accurately predict the hydrolysis index of the gluten-free cookies owing to their higher coefficient of determinant (R^2 > 0.9). The predictive capability assessment of response surface methodology and support vector machine revealed the superiority of support vector machine (0.9658, 0.9329, 0.059) in predicting the hydrolysis index of the gluten-free cookies over response surface model (0.9613, 0.9241, 0.063) owing to its high correlation coefficient (R), Coefficient of determinant (R^2) and lower mean square of error as well as root mean square of error (RMSE).

Keywords: *Gluten-free cookies; Hydrolysis index; Starch digestibility; Mathematical modelling; Machine learning*

1. Introduction

Recently, there had been an increase in people with celiac diseases, an immune-mediated enteropathy disease arising for the ingestion of food products containing gluten in people genetically susceptible to it. The increase in celiac disease had led to an increasing demand for gluten-free diets or products. This disease is common among westerners and had been reported low in Africa due to improper health facilities to diagnose the disease. Although, many approaches had been used in the treatment of the disease, the only proven treatment is the removal of gluten and prolamins or its precursors such as hordeins in barley, secalin in rye, and avenins in oats from genetically susceptible person's diets. This had led to the development of gluten-free products by several researchers from diverse crops such as Vicia faba bean (Schmelter *et al*., 2021), rice flour (Rocchetti *et al*., 2019), pseudo-cereal (Martínez-Villaluenga *et al*., 2020) and plantain flour (Gutiérrez, 2018). These crops however, have both commercial and other industrial values, thereby contributing to the high cost of production of gluten-free products (Olawoye et al., 2017). Hence the need to search for a local alternative amongst the under-utilized crop from which the product can be produced, hence, *cardaba* banana.

Cardaba banana also known as cooking banana is a breed of Musa spp usually cultivated in sub-Sahara Africa. It is widely known for its high starch content (81.84%) in which amylose is made up of 31-35% of the starch composition thereby making it suitable as a diet in the management of diabetes Mellitus; a disease that arises from glucose absorption malfunction. The application of the cooking banana is limited due to its high perishability when ripe and unlike dessert banana, it found no usage after ripening. Due to this, it had found application in the production of complementary food (Ayo-Omogie & Ogunsakin, 2013) as well as functional starch (Olawoye *et al*., 2020a; Olawoye *et al*., 2020c). However, because the cooking banana contains no gluten, it serves as good raw material in the production of gluten-free products.

In the production of gluten-free cookies, the choice of raw materials and their composition are important as they affect the physical, chemical and nutritional characteristics of the final product. One important component of the raw material that affect these is the carbohydrate (starch) composition. Starch is a polymeric aldehyde join together by an alpha 1-4 glycosidic bond in an unbranched chain and a beta 1-6 glycosidic bond in branched chain. During food digestion, starch is broken down in the human gastrointestinal tract by alpha-amylase into glucose which is the main source of biofuel in humans. However, high glucose in human blood resulted in complications arises from type 2 diabetes. To solve this problem, it is necessary to control the amount of glucose in food to produce gluten-free cookies with a low glycemic or hydrolysis index; which is the response of the body to blood glucose after two hours of the consumption of carbohydrate food. Hence, the need for statistical modelling and optimization of the process variables for the production of the low glycemic or hydrolysis index gluten-free cookies.

Statistical modelling and optimization had been widely used for the prediction and analysis of chemical reactions or processes. Of the approaches used in mathematical modelling, data-driven modelling focuses on input-output functionality findings from experimental data set obtained in the chemical process. This approach helps in predicting outcomes and finding the optimum condition of process variables that will bring about the targeted goal. Olawoye and Kadiri (2016) use the response surface methodology approach in modelling the antioxidant properties of grain amaranth flour. Using this approach, they were able to optimize the process parameters for optimal antioxidant activities. Support vector machine is a machine learning algorithm that provides good prediction accuracy, owing to its tolerance to erroneous and noisy data. Its application in food process operation is limited (Saha & Manickavasagan, 2021) and hence its usage in this study. This study aims at statistical modelling of the hydrolysis index of gluten-free cookies using response surface methodology and support vector machine.

2. Material and Methods

2.1. Materials

The main raw materials used for the production of gluten-free cookies are *Cardaba* banana flour and starch flour. Other ingredients in the production of the cookie were obtained from a local supermarket in Ile-Ife, Osun State, Nigeria. Chemicals used for the analysis were of analytical grade and were obtained from Sigma-Aldrich, USA.

2.2. Starch extraction from *cardaba* banana

The starch extraction was carried using the procedure described by Olawoye *et al*. (2020c). Briefly, the banana was washed and peeled underwater to avoid enzymatic browning of the peeled banana. The peeled banana was cut into smaller sizes and was milled mechanically using a Stephan milling machine (Germany). Following milling, the starch mash was diluted with water (1:10) and was passed through a sieve (200 um mesh size). The subsequent starch slurry obtained was washed with water three times and was left for 8 hours for the starch to settle down. This was followed by decanting the water and the starch obtained therein was dried at 40 °C for 8 hours and kept inside an airtight container under refrigeration before use.

2.3. Modification of *cardaba* banana starch using citric acid.

Cardaba banana starch produced was modified using citric acid modification following the methodology of Klaushofer *et al*. (1978) as modified by Olawoye and Gbadamosi (2020).

2.4. Gluten-free cookie production

The cookie production was carried out using the method described by Giuberti *et al*. (2015). Briefly, citric acid modified *cardaba* banana starch was blended with cardaba banana flour (80:20 w/w). Buttercream (8.5 w/w of flour blend) and whole egg (12 w/w of flour blend) were mixed and was added to the already pre-mix flour blend in an electric mixer (Kenwood KMM021, UK). The ingredients were thoroughly mixed for 7 minutes to form a homogenous dough. After mixing, the dough was flattened using a roller and was stored in refrigeration (4 °C) for 30 mins. The dough cutter was used to cut the flattened dough into small sizes and were baked at various baking temperature and time following the central composite design shown in Table 1.

Table 1: Experimental design for process variables

Independent variables	Codes	Range and level				
		-α	-1	0	+1	+α
Baking Temperature (°C)	A	135	150	165	180	195
Baking Time (min)	B	5	10	15	20	25

2.5. In vitro starch digestibility of the gluten-free cookie

The in vitro starch digestibility, as well as the digestion kinetics, was done using the method described by Olawoye *et al*. (2020b). The glucose released was evaluated using the colourimetric method described by Olawoye and Gbadamosi (2020) while the starch released was quantified as the percentage starch release at a different time. The Hydrolysis index was calculated from the relationship between the area under curve (AUC) (0 – 180 min) for the cookie and AUC for white bread as described by Goni 1997. The equation for the hydrolysis index (HI) of the cookie is presented below.

$$\mathbf{AUC} = C_{\infty}(t_x - t_0) + \frac{C_{\infty}}{k}\left(e^{-ktx} - e^{-kt0}\right) \qquad \text{Eq. (1)}$$

$$\mathbf{AUC} = 180\, C_{\infty} + \frac{C_{\infty}}{k}\left(e^{-180k} - 1\right) \qquad \text{Eq. (2)}$$

Hydrolysis index (HI) was calculated as the relationship between the Area under Curve (AUC) for a test food and AUC for a reference food (White bread), expressed as a percentage (Granfeldt et al., 1992).

$$\textbf{HI} = \frac{Total\ Glucose\ from\ 100g\ cooked\ sample\ (on\ a\ dry\ basis)\ at\ 120\ min}{total\ Glucose\ from\ 100\ g\ white\ bread\ (on\ a\ dry\ basis)\ at\ 120\ min} \qquad \text{Eq. (3)}$$

2.6. Modelling using support vector machine

Support vector machine is a machine learning algorithm based on Vapnik-Chervonenkis dimension theory (Bisgin et al., 2018). It is a learning algorithm that utilizes a structural risk minimization (SRM) induction principle to profound a unique solution to the experimental data set. SVM exhibits high prediction efficiency over other statistical modelling tools by recognizing a non-linear relationship between the dependent and independent variables. Also, support vector machine - regression poses an advantage over other machine learning tools in that a small number of parameters are required; the kernel type as well as cost parameter C which indicates the balance in the tolerance for training errors and generalization capability. In this study, SVM was applied purposely to correlate the hydrolysis index of the gluten-free cookie with the independent variables (baking temperature and baking time). The data set from the Central composite design were used for the support vector machine (regression). The experimental data were randomly divided into two; 80% of the data was used as training data set while the remaining (20%) was used as the testing data set to predict the hydrolysis index. For the modelling operation, the radial basis function kernel was selected and was characterized by the equation below.

$$Y(x) = \sum_{n=1}^{N} w_n K(x, x_n) + w_0 \qquad (4)$$

Where w_n is the model weight and $K(x.x_n)$ is the kernel function

2.7. Performance analysis of the RSM and SVM model

The performance of the model (RSM and SVM) in predicting the hydrolysis index of the gluten-free cookies was evaluated using some fit statistics cateria such as correlation coefficient (R), coefficient of determinant (R^2), adjusted R^2, mean square of error, root mean square of error, average absolute deviation (AAD) and standard error of prediction (SEP).

3. Result and discussion

3.1 Analysis of the RSM model of hydrolysis index

The result of the hydrolysis index of the cookies obtained from a central composite design of response surface methodology is shown in Table 2. The result revealed that the hydrolysis index ranged from 56.04 to 56.79 for actual value and between 56.04 - 56.82 for predicted value. The values obtained in this study were, however, lower than the values obtained by Giuberti *et al*. (2016) for cookies made from waxy rice starch. The lower HI values could be attributed to the citric acid modification of the *cardaba* banana starch before use. Citric acid modification of starch had been reported to slow down enzymatic digestion of starch thereby, yielding a low hydrolysis index (Remya et al., 2018). To ascertain the relationship between the independent variables (baking temperature and baking time) and dependent variable (hydrolysis index), a second-order polynomial model was used and the relationship is presented using equation 5 below. The second-order polynomial model was subjected to analysis of variance and the result is presented in Table 3.

HI = 56.4997 + -0.177778 * A + -0.0565693 * B + -0.0658922 * AB + -0.0264931 * A^2 + 0.0514742 * B^2 (5)

Table 2. Experimental and predicted values of hydrolysis index of GF cookies

Run	Independent variables		Hydrolysis index		
	Temperature (°C)	Time (min)	Actual	RSM predicted	SVM predicted
1	165	25	56.60	56.59	56.56
2	165	15	56.46	56.50	56.43
3	135	15	56.73	56.75	56.76
4	165	5	56.79	56.82	56.76
5	150	10	56.74	56.69	56.75
6	165	15	56.65	56.50	56.63
7	180	20	56.21	56.22	56.28
8	165	15	56.39	56.50	56.53
9	180	10	56.49	56.47	56.43
10	195	15	56.04	56.04	56.08
11	165	15	56.50	56.50	56.53
12	165	15	56.46	56.50	56.53
13	150	20	56.73	56.71	56.69

Table 3: Analysis of variance of hydrolysis index of the GF cookies

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	0.5379	5	0.1076	17.22	0.0008	significant
A-Baking Temperature	0.3793	1	0.3793	60.71	0.0001	
B-Baking Time	0.0384	1	0.0384	6.15	0.0423	
AB	0.0174	1	0.0174	2.78	0.1394	
A^2	0.0161	1	0.0161	2.57	0.1527	
B^2	0.0607	1	0.0607	9.72	0.0169	
Residual	0.0437	7	0.0062			
Lack of Fit	0.0046	3	0.0015	0.1553	0.9210	not significant
R^2	0.9248					
Adjusted R^2	0.8711					
Predicted R^2	0.8332					
Adeq precision	14.53					
CV (%)	0.14					

The ANOVA result revealed that the model for the experimental design is significant owing to the p-values less than 0.05. Aside from the experimental design model, it could also be seen that among the model terms, only the interaction term of the independent variables, as well as the quadratic term of the baking temperature, were not significant ($p > 0.05$). The linear term of the baking temperature of the gluten-free cookie was the most significant among the model terms, evident of its very low p-value (0.0001) and high Fisher's test value (60.71). The Pareto chart (Figure 1) shows the relationship between the process parameters as well as the response (hydrolysis index). As could be seen in the chart, the bar chart that crosses the reference indicates significant terms while those below the reference line are not significant in the determination of the hydrolysis index of the gluten-free cookies. The regression coefficient revealed that only the quadratic term of the baking time had a positive value and hence, a positive relationship with the hydrolysis index while others had a negative relationship with the hydrolysis index.

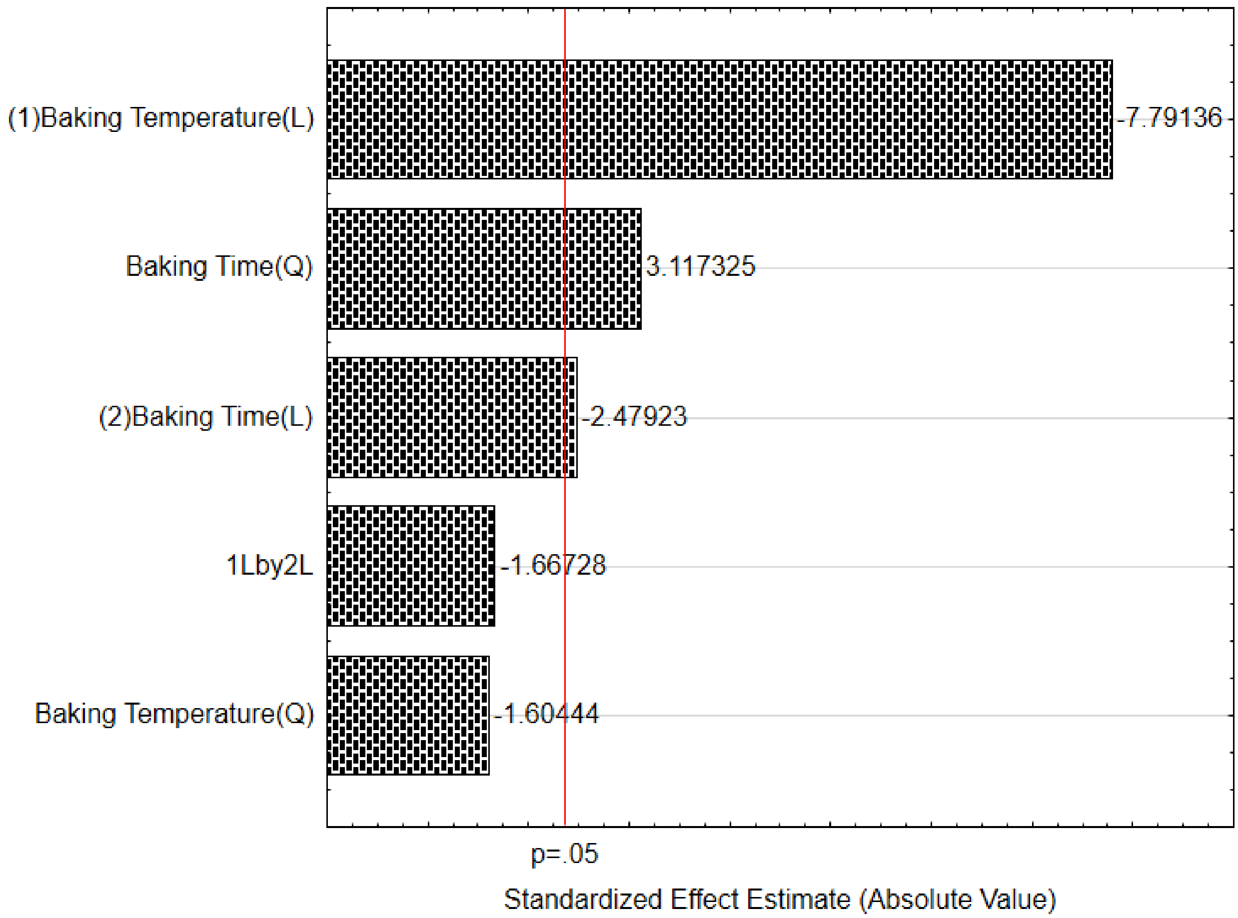


Figure 1: Pareto chart for hydrolysis index of the GF cookies

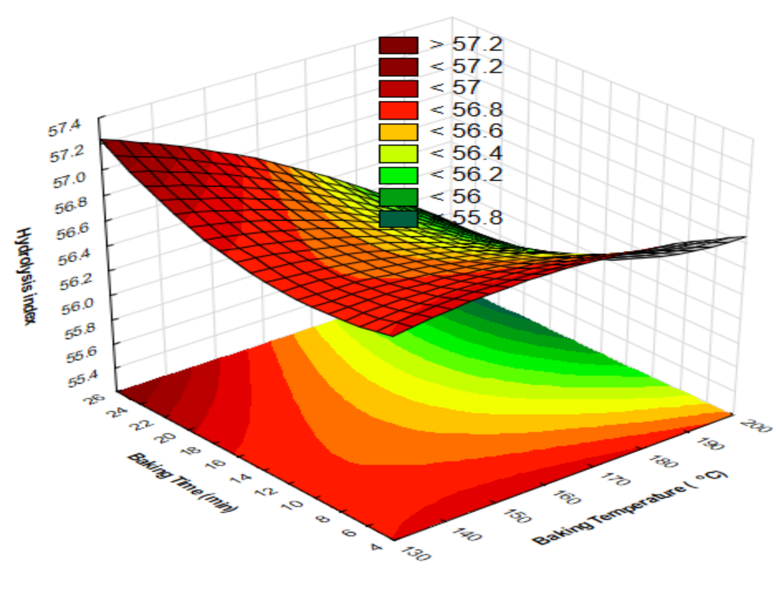
The goodness of fit of the model was evaluated using analysis of variance and presented in Table 3. The lack-of-fit obtained for the experimental model is 0.9210 which implies that it is not significant ($p > 0.05$) in relation to the pure error. The high lack-of-fit indicate there is a 92.10% chance that the lack-of-fit was due to noise. A non-significant lack-of-fit affirm the goodness of fit of the experimental model. Also, the coefficient of determinant (R^2) of 0.9248 is an indication that 92.48 of the variation in the experimental data could be accounted for by the independent variable while only 7.52% of the variation can't be accounted for. According to Morakinyo *et al*. (2021), an R-square value above 0.80 is a reflection of the significance of the model. The R-square alone, however, does not reflect the goodness of fit of the model because when a new model term is added to the experimental design, its effect is not being accounted for (Odejobi *et al*., 2018). Hence, the adjusted R-square which take into consideration the effect exhibited when a new independent variable is added was 0.8711. Unlike the coefficient of determinant, the adjusted r-square only increase when a new model term is added to the experimental design. Finally, the adequate precision which also measures the goodness of fit of the model is 14.53. This is a measurement of the signal to noise ratio. A value of above 4 is desirable and the ratio of 14.53 indicates an adequate signal.

3.2. Effects of baking temperature and time on hydrolysis index

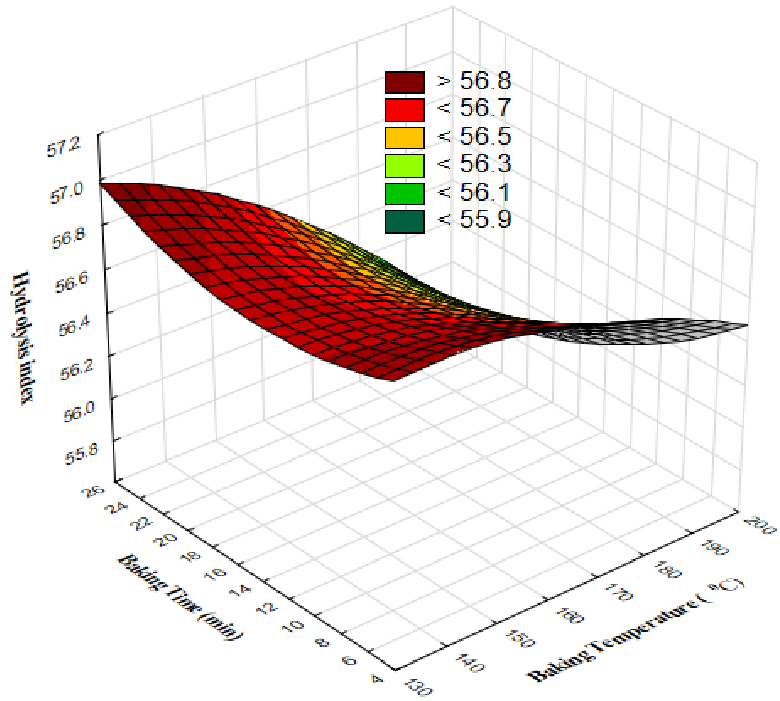
The effect of the processing variables (baking temperature and time) on the hydrolysis index of the gluten-free cookies is shown in Figure 2. The 3-D surface plot shows that both the baking temperature and baking time had a linear effect on the hydrolysis index. At constant, an increase in the baking temperature resulted in a decrease in the hydrolysis index of the gluten-free cookies. An increase in the baking time up 16 mins at a low baking temperature on the other hand resulted in an initial decrease in the hydrolysis index of the cookies. This, however, increases as the baking time progresses above 16 mins. Baking for a long period increases the rate of gelatinization of starch as a result of an increase in the cookies core temperature. This, however, upon cooling of the cookie enhance retrogradation of the starch and hence, limit the hydrolysis index of the cookie. An increase in the baking temperature at an elevated temperature resulted in a significant decrease in the hydrolysis index. This could be due to the formation of complexes between lipids and starch (amylose) at a high temperature which in turn result in low digestibility of the cookie and hence, low hydrolysis index. For health benefits, the hydrolysis index must be at the barest minimum possible (Olawoye et al., 2020). To achieve this, the baking temperature, as well as the baking time, must be at their highest value.

3.3. Modelling hydrolysis index using support vector machine

Support vector machine, a pattern classification technique which unlike the traditional method of modelling minimizes experimental data training error by maximizing boundary separation between the training data set and hyperplane. To model the hydrolysis index of the cookie using SVM, the experimental data obtained from the central composite design were used. The data were divided into two in which 75% of the data set was used as training data while the remaining data set were used as testing data which was used in data prediction. The kernel function selected for the modelling operation was the RBF kernel in which parameters C (error penalty) and Ɛ (epsilon) were carefully chosen as they influence the final model prediction performance.



(a)



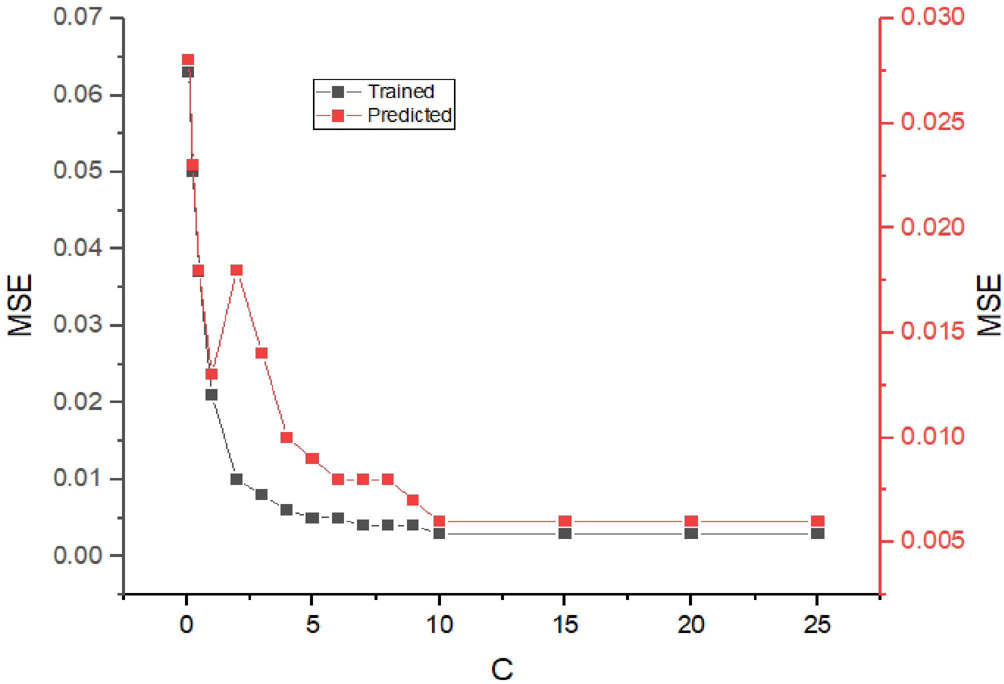
(b)

Figure 2: Effect of processing parameters on hydrolysis index of the GF cookies: (a) RSM; (b) SVM

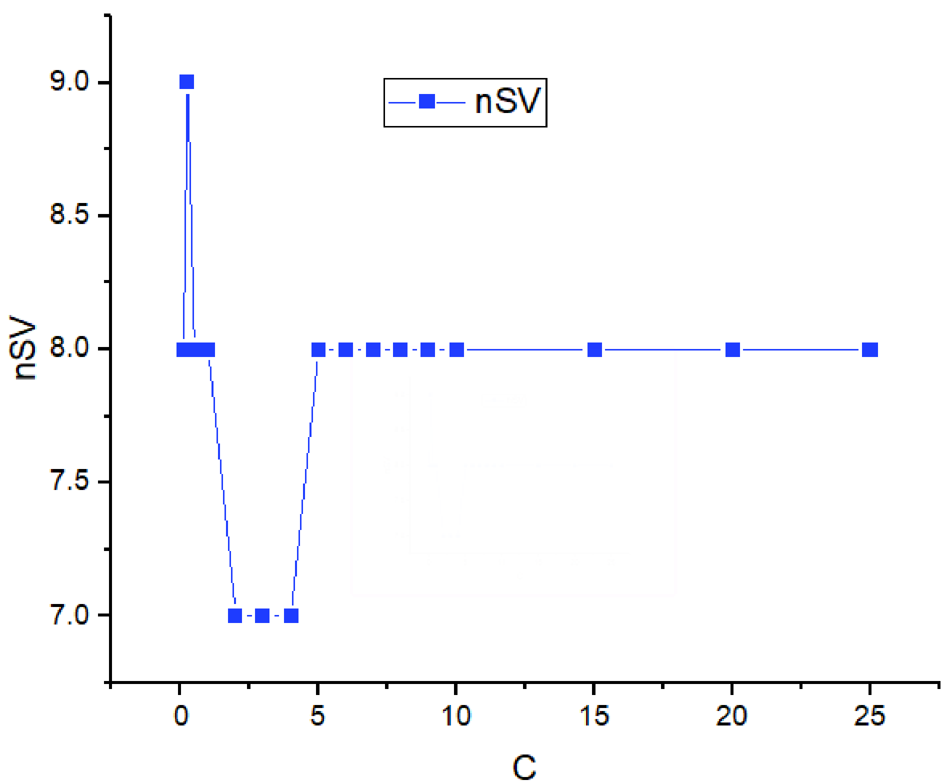
3.4 Selection of the SVM parameters (C and ε)

Selection of C

The parameter C also known as error penalty functions in adjusting the ratio of the learning machine interval and the empirical risk. When the value of C is small, then the empirical error penalty is small which also result in the complexity of the learning machine being small (Shao et al., 2020) and hence the over-learning of the SVM model and vice-visa. Also, when C is too large or too small, it affects the performance of the SVM model. Therefore, in this study, the SVM parameter ε was fixed at 0.1while the error penalty (C) was varied between 0.1 to 25 for the training of the SVM model using central composite design datasets. The result obtained was the mean square of error as well as the number of support vectors, it was recorded as is shown in Figure 3. As it could be seen from Fig. 3, the MSE of the trained and predicted dataset firstly decrease largely as the value of C increases and remain constant when the value of C is 10 and above. The number of support vectors falls sharply and remain constant as C equals 5, it then increases when C was increased to 6 and remain constant throughout the value of C. From this result, 10 was chosen for the value of C.



(a)

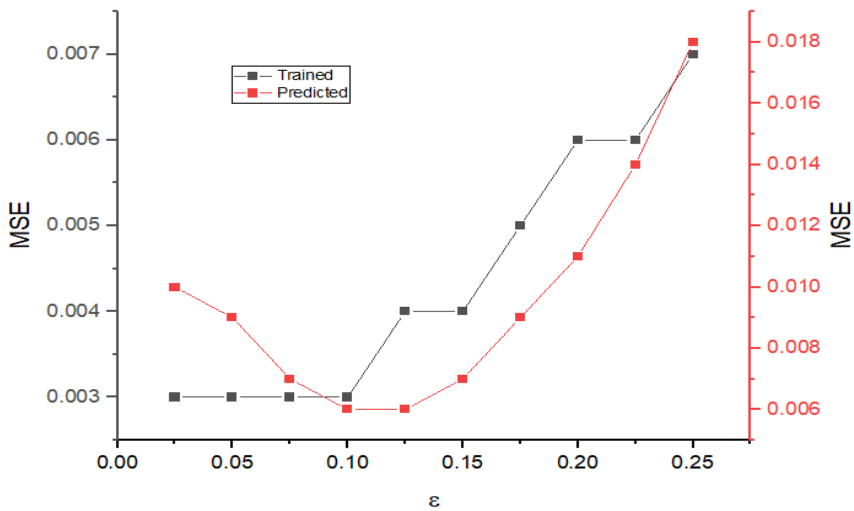


(b)

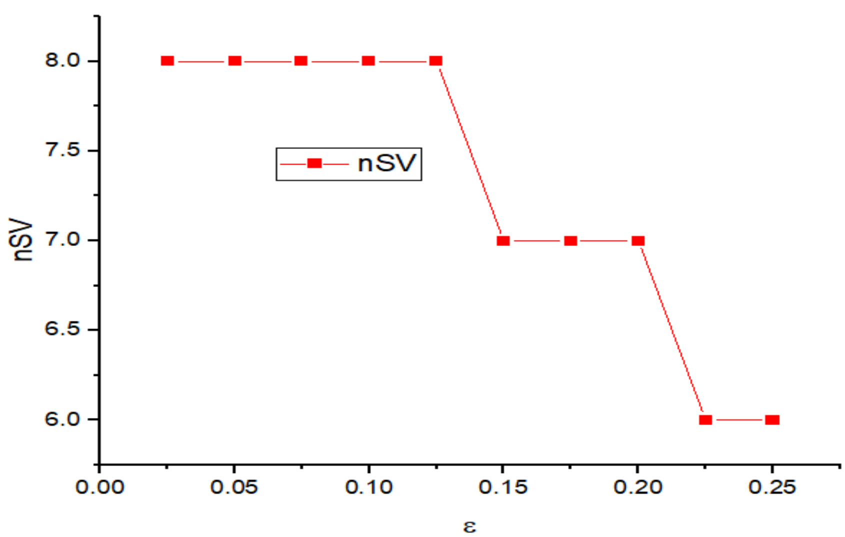
Figure 3: The result of various C, where Ɛ = 0.01: (a) MSE (b) nSV

Selection of ε

The selection of ε is important as it influences the performance of the SVM model. When ε increases continuously, the ability of the model to learn the datasets decreases, the empirical risk increases, while the ability of the model to predict the dataset decreases owing to insufficient learning by the model (Shao et al., 2020). For an optimal selection of ε, the C parameter was fixed at a constant value of 10 while ε was set at various values ranging between 0.025 and 0.25. The result while including the MSE of the trained and predicted data as well as the number of support vectors is shown in Figure 4. From Figure 4, it could be seen that the MSE value of the trained dataset remains constant at first followed by a steady and gently increase as the value increases above 0.1. The MSE value of the predicted dataset decreases slightly and reached a minimum at ε equals 0.1, it then increases slightly as e increases above 0.1. However, the number of vectors remain constant as E increased to 0.125, it was preceded by a sharp decrease in nSV when E increase from 0.125 to 0.15. Based on the value of prediction error as well as the number of vectors obtained in Fig 4., ε was chosen to be 0.1.



(a)



(b)

Figure 4: The result of various Ɛ, where C = 10: (a) MSE (b) nSV

3.5 Prediction of hydrolysis index using SVM

To predict the hydrolysis index of the gluten-free cookies, the dataset was divided into two in which 75% of the datasets were used to train the model while 25% was used in predicting the hydrolysis index of the cookie. Since the performance of the SVM model in predicting the hydrolysis index is dependent on the SVM parameter C and E, the parameters were set at their optimal value of 10 and 0.1 for C and E, respectively based on their MSE value. The predicted hydrolysis index was obtained using cross-validation and it is as presented in Table 4 while the coefficient of determinant, as well as the mean square of error of the SVM model, were 0.9658 and 0.004, respectively. These values confirm the feasibility and accuracy of the SVM model in predicting the hydrolysis index of the cookie.

Table 4: Predictive capability evaluation of RSM and SVM in predicting hydrolysis index

Parameters	RSM	SVM
R	0.9613	0.9658
R^2	0.9241	0.9329
Adjusted R^2	0.9172	0.9268
MSE	0.004	0.003
RMSE	0.063	0.059
AAD	0.067	0.083
SEP	0.112	0.105

3.6 Performance analysis of RSM and SVM model

The performance analysis of the RSM and SVM model in predicting the hydrolysis index of the gluten-free cookies was evaluated using correlation coefficient, R^2, adjusted R^2, MSE, RMSE, AAD and SEP. The result of the analysis observed showed that the R, $R^{2,}$ and adjusted R^2 were found to be sparingly higher in the SVM model compared to the RSM model (Table 4). The MSE, RSME, AAD and SEP were however found to be low for both models, however, the MSE, RMSE and SEP were low for the SVM model in comparison to the RSM model. This finding is an indication of the superiority of the support vector model in predicting the hydrolysis index of the gluten-free cookies over the response surface model. The superiority of the SVM model over RSM was further affirmed by plotting the actual experimental value, RSM and SVM predicted value against the experimental runs and it's shown in Figure 5. From the plot, it could be seen that the actual hydrolysis index values were superimposed on the predicted values obtained using the SVM model while RSM predicted values swerve away from the observed values.

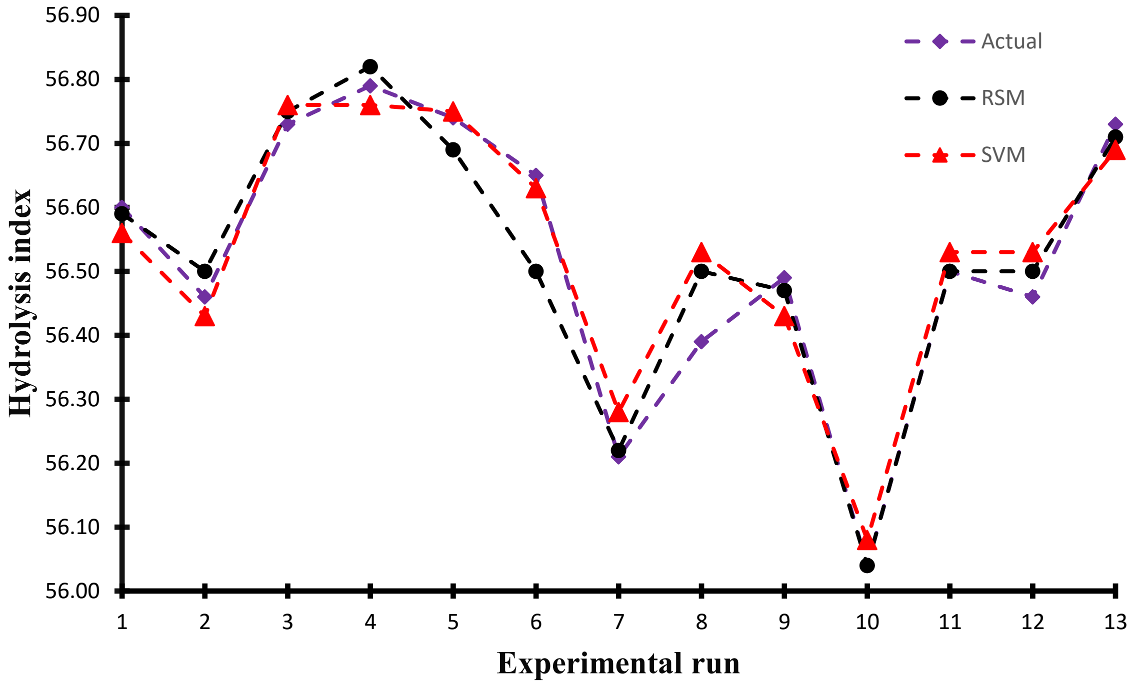


Fig. 5. Comparison between predicted HI (RSM and ANN) against experimental HI

4 Conclusion

In this study, the hydrolysis index of gluten-free cookies made from *cardaba* banana was statistically modelled using response surface methodology and support vector machine. The experimental design was based on a central composite design. The mathematical modelling revealed that both modelling approaches (response surface methodology and support vector machine) accurately predicted the hydrolysis index of the gluten-free cookies owing to their higher coefficient of determinant (R^2 > 0.9). The predictive capability assessment of response surface methodology and support vector machine revealed the superiority of the support vector machine in predicting the hydrolysis index of the gluten-free cookies over the response surface model. The result obtained is an indication that the flour and starch of under-utlized *cardaba* banana could served as an important raw material in the production of gluten-free cookies with low hydrolysis index for coeliac and diabetes patients.

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