
Modeling the Migration of 2,6-di-tert-butyl-p-cresol from Plastic Bags into *attiéké* (Cassava Couscous) from Physico-Chemical and Morphometric Parameters

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Abstract: *Attiéké*, couscous made from fermented cassava, is a staple food in Côte d'Ivoire packaged in polythene plastic bags. The antioxidant BHT was analyzed both in the plastic bags and in the *attiéké* at different temperatures and at different levels inside the *attiéké* ball. A modelling study was conducted to determine a quantitative relationship between the BHT concentration in the *attiéké* and the descriptors which are the concentration of BHT in the plastic bag, grain size, depth (from the surface to inside the *attiéké* ball), duration and conditioning temperature of the *attiéké* in the plastic bags. BHT, initially not detected in the *attiéké*, migrates there depending on the packaging temperature of this commodity and certain parameters. This study was conducted by using multiple linear regression. A quantitative model was proposed. The statistical indicators revealed effective predictions with the determination coefficient equal to 0.92 and the standard error equal to 0.191. The value of the Fischer test was 170.250 and the cross-validation determination coefficient was 0.9136. The results obtained suggest that the combination of the descriptors used could be useful in predicting *attiéké* contamination by plastic bags. Temperature is the most important descriptor for predicting the BHT concentration in the *attiéké* with a normalized coefficient equal to 0.846 followed by depth (from the surface to inside the *attiéké* ball) (-0.822).

Keywords: Modelling, Migration, *attiéké*, BHT, Plastic Bags, Physico-Chemical Descriptors

1. Introduction

BHT (2,6-di-tert-butyl-p-cresol) is a substance used as an antioxidant in plastic bags. It belongs to the group of hindered phenol antioxidants. Antioxidants are used to prevent discoloration, lack of flexibility and strength of the plastic polymer [1]. This compound is one of the endocrine disruptors [2]. Varuna *et al.* have demonstrated that BHT has a hepatotoxic effect [3]. Unfortunately, this substance can contaminate the *attiéké* during its packaging in plastic bags. *Attiéké* is a couscous produced from the fermentation of

cassava. It is a staple food in Côte d'Ivoire. Its annual production is estimated between 18,965 tons and 40,000 tons [4]. According to European Union Regulation EC No. 10/2011, the specific migration limit (SML) for BHT is 3 mg/Kg [5]. The quantification of plastic bag additives in the *attiéké* is a long and costly process in terms of the equipment used and the chemicals. To overcome its difficulties, alternative methods for predicting food contamination with BHT are proposed. Modeling is one of the approaches used to study the migration of contaminants in food or food simulants. Based on the Quantity-Structure-Property

Relationship (QSPR) or Quantity-Structure-Activity Relationship (QSAR), a predictive model based on physico-chemical descriptors was determined [6, 7]. This statistical approach allows the use of methods such as linear regression, non-linear regression.

A statistical model is a simplified and quantified representation of a phenomenon. It leads us to a better understanding of reality and even make predictions. It allows, through mathematical equations involving parameters, to explain or predict a variable (dependent variable or variable to be explained) by explanatory variables (independent variables) [8]. Traistaru *et al.* developed a statistical prediction model to determine global migration (dependent variable) from temperature and time (independent variables) in food simulants [9]. Musoke *et al.* studied the migration of chemical contaminants from polyethylene bags into food during cooking [10]. For the time being, no reference is found about the migration of pollutant in *attiéké*. So, it is interesting to develop a mathematical model to predict the migration of pollutant in a solid food like *attiéké*.

The general objective of this work is to determine a statistical model using multilinear regression capable of predicting the transfer of the additive (BHT) into the *attiéké* packaged in plastic bags from morphometric (grain size and different levels within the *attiéké* ball) and environmental variables related to its packaging. In particular, it is necessary to identify explanatory and relevant variables favourable to the transfer of the pollutant in order to generate the mechanisms for better quality packaging of *attiéké* for good consumer health.

2. Material and Methods

2.1. Material

The study material consists of *attiéké* packaged in plastic bags sold in shops. The modeling was carried out using the multilinear regression method implemented in the Excel tables [11, 12].

2.2. Sampling

Three-stage cluster sampling method was used. At the primary level, the three cities of southern Côte d'Ivoire, Dabou, Jacqueline and Abidjan, known as the main *attiéké* producing cities [4]. At the secondary level, four municipalities in the city of Abidjan (Abobo, Attécoubé, Cocody, Marcory), 1 village in the city of Dabou and 1 village in the city of Jacqueline. *Attiéké* production sites constitute the tertiary level [4]. The normal *attiéké* "small grain" was collected from production sites in Dabou, Jacqueline and Aboboté in the municipality of Abobo. As for the "big grain" *attiéké* called «*agbodjama*», it was collected from production sites in Anono in the commune of Cocody, Anoumambo in the commune of Marcory and Abobodoumé in the commune of Attécoubé. At each site, approximately 200g of *attiéké* were collected. Samples were

taken at 70°C, 60°C, 50°C, 40°C and 30°C. For each temperature, 9 samples were taken and packaged in plastic bags from 3 different plants. After each conditioning period (1 hour, 2 hours and 3 hours), using stainless steel pliers, 5 g of *attiéké* were collected at different depth levels of the *attiéké* ball: at the surface (up to 0.5 cm), at 1 cm and at 1.5 cm. A total of 45 *attiéké* balls were collected from each site and 270 *attiéké* balls were collected from all 6 sites. The control consists of the *attiéké* taken under the same conditions and introduced into a brown glass vial [13].

2.3. Antioxidant BHT Analyses

The analyses were performed by high performance liquid chromatography using the method described by Kombo *et al.* [14].

2.4. Physico-chemical Descriptors

The concentration of additives migrating from plastic bags in the *attiéké* might depend on several parameters. According to Musoke *et al.*, the migration of chemical contaminants from polyethylene bags to food depends on temperature, duration and depth level (from the surface to the interior of the food) [10]. It is essential to calculate or measure a large number of different descriptors in order to determine which ones are the most relevant to the established model. Each model is based on a number of descriptors used by the latter. According to Topliss and Edwards and according to Ghamadi *et al.*, the maximum number of descriptors used should be about one-fifth of the number of learning game observations included in the model [15, 16]. A method for selecting the explanatory variables, including step-by-step method, was carried out. The latter consists in incorporating the variables into the model one by one by selecting at each step, the variable whose partial correlation with the modelled quantity allow to increase the determination coefficient (R^2). At each step, the significance of the partial correlations of the previously introduced variables is verified [16]. Thus, several descriptors that may influence the migration of pollutants are used to predict the concentration of contaminants in the *attiéké*.

The descriptors considered in this study are: the concentration of BHT in the plastic bag, the size of the grains, the depth level (from the surface to inside the *attiéké* ball), the duration and temperature of conditioning of the *attiéké* in the plastic bags. Temperature is one of the most important kinetic factors in the mechanisms for transferring pollutants from one matrix to another. It plays a fundamental role in the kinetics of physico-chemical and biological reactions as well as the value of equilibrium constants [17].

2.5. Estimation of the Predictive Capacity of a Model

The concentration of BHT in *attiéké* was presented by 120 study samples with a concentration range from 1.01 to 3.46 mg/kg. This range of concentrations with reduced variation makes it possible to define a better quantitative

relationship between the concentration of BHT in the *attiéké* and the physico-chemical descriptors of the samples taken. The quality of the model is determined by taking into account various statistical indicators such as the determination coefficient (R^2), standard error (RMSE), Fischer test (F) and cross-validation determination coefficient (Q_{CV}^2). These indicators provide information on the adjustment of theoretical and experimental values. They allow the quality of the model to be assessed and its accuracy to be expressed [18]. The determination coefficient R^2 gives an evaluation of the dispersion of the calculated values around the experimental values. The quality of the model is better when the points evaluated by R^2 are close to the adjustment line. The determination coefficient (R^2) is given by the expression:

$$R^2 = 1 - \frac{\sum(y_{i,exp} - \hat{y}_{i,theo})^2}{\sum(y_{i,exp} - \bar{y}_{i,exp})^2} \quad (1)$$

The standard error or standard deviation (RMSE) is used to assess the reliability and accuracy of the model. Its expression is as follows:

$$RMSE = \sqrt{\frac{\sum(y_{i,exp} - \hat{y}_{i,theo})^2}{n-k-1}} \quad (2)$$

Concerning the Fischer F test, it is useful for the choice of the model's constituent descriptors. The Fischer test is given by the mathematical equation:

$$F = \frac{\sum(y_{i,theo} - y_{i,exp})^2}{\sum(y_{i,exp} - y_{i,theo})^2} * \frac{n-k-1}{k} \quad (3)$$

The coefficient for determining the cross-validation is obtained by the equation :

$$Q_{CV}^2 = \frac{\sum(y_{i,theo} - \bar{y}_{i,exp})^2 - \sum(y_{i,theo} - y_{i,exp})^2}{\sum(y_{i,theo} - \bar{y}_{i,exp})^2} \quad (4)$$

In these equations, k is the number of descriptors, n is the number of observations of the test set and n-k-1 is the degree of freedom [19].

$y_{i,exp}$ is the experimental value of the BHT concentration of the *attiéké*, $\hat{y}_{i,theo}$ is the theoretical value of the BHT concentration in the *attiéké* and $\bar{y}_{i,exp}$ the experimental mean value of the BHT concentration in the *attiéké*.

2.6. Statistical Analyses

2.6.1. Principal Component Analysis (PCA)

Principal Component Analysis is a data analysis tool that aims to explain the structure of correlations or covariances. It uses linear combinations of the original data and allows the data to be interpreted (Soro *et al.*, 2018). In this study, the PCA was used not only to assess the relationships between the different variables measured, but also to correlate the physico-chemical descriptors obtained with the concentrations of BHT migrating from plastic bags to *attiéké*.

2.6.2. Multiple Linear Regression (MLR)

Multiple linear regression is a statistical method that can be used to determine a relationship between the dependent variable and several independent variables (descriptors). This statistical method minimizes the differences between actual and predicted values. It also makes it possible to identify the most influential descriptors. It is the most widely used tool for studying multidimensional data. It is based on the y function of the XLSTAT statistical software whose equation is of the form:

$Y = a + (bx_1 + cx_2 + dx_3 + ex_4) + (fx_{12} + gx_{22} + gx_{32} + hx_{42})$ where a, b, c, . . . represent the parameters and x_1, x_2, x_3, \dots variables.

The quality of the model developed depends on its validation. Indeed, in order to estimate its predictive power, additional experimental data are essential [16]. The MLR was determined using the XLSTAT statistical software version 2014.

2.6.3. Reporting of Predicted and Experimental Data

From the validation set, the model is acceptable when the relationships between theoretical and experimental values are close to unity [6].

2.7. Criteria for Accepting a Model

The more strongly the experimental values are correlated with the theoretical values, the closer the determination coefficient (R^2) is to one (1).

$|R^2 - R^2_{adj}| \leq 0.3$, translates that the number of descriptors involved in the model is acceptable. A predictive model is acceptable when the RMSE is less than 0.3. However, the excellent values of R^2 and RMSE are not sufficient to validate a good model. Additional indicators such as the cross-validation determination coefficient Q_{CV}^2 are required to determine the predictive capability of a model.

A predictive model is considered good when $|R^2 - Q_{CV}^2| < 0.3$ [21].

A model is considered good if $Q_{CV}^2 > 0.5$ and excellent if $Q_{CV}^2 > 0.9$ [22].

3. Results

3.1. BHT Analysis Results

Eighty (80) samples used to calibrate the model (learning or test set) and the other 40 samples used to validate it (validation set) are recorded in Table 1. In this study, there are 5 descriptors. Table 1 presents the concentrations of BHT in *attiéké* ($C_{BHT,Attiéké}$) according to different descriptors. The concentration of BHT in *attiéké* varies from 1.01 to 3.46 mg/kg. $C_{BHT,Sachet}$ is the concentration of BHT in plastic bags in mg/Kg, T_{grain} is the size of the *attiéké* grains in mm, T is the packaging temperature of the *attiéké* in degrees Celsius (°C), D is the packaging duration in hours and P is the depth level of the *attiéké* ball in cm (from surface to inside *attiéké* ball).

Table 1. BHT concentrations according to the different descriptors.

Observation	C _{BHTsachet}	T _{grain}	T	D	P	C _{BHTattiéké}	Observation	C _{BHTsachet}	T _{grain}	T	D	P	C _{BHTattiéké}
Training set													
1	26	1,1	70	1	0,5	3,13	41	18	1,1	70	3	0,5	3,12
2	26	1,1	70	1	1	2,32	42	18	1,1	50	2	0,5	1,69
3	26	1,1	70	2	0,5	3,34	43	18	1,3	70	1	0,5	3,01
4	26	1,1	70	2	1	2,56	44	18	1,3	70	2	0,5	3,11
5	26	1,1	60	2	1	1,63	45	18	1,3	50	2	0,5	1,91
6	26	1,1	60	3	0,5	2,93	46	18	1,3	50	3	0,5	1,97
7	26	1,1	60	3	1	1,66	47	18	0,8	70	1	0,5	3,04
8	26	1,1	40	1	0,5	1,53	48	18	0,8	70	3	1	2,32
9	26	1,1	40	2	0,5	1,93	49	18	0,8	60	1	0,5	2,57
10	26	1,3	70	2	1	2,13	50	18	0,8	60	3	1	1,48
11	26	1,3	70	3	0,5	3,41	51	18	2,4	70	2	0,5	3,19
12	26	1,3	70	3	1	2,16	52	18	2,4	70	2	1	2,06
13	26	1,3	60	1	1	1,5	53	18	2,4	70	3	1	2,15
14	26	1,3	60	3	0,5	2,88	54	18	2,4	60	1	0,5	2,23
15	26	1,3	60	3	1	1,66	55	18	2,4	60	2	0,5	2,28
16	26	1,3	50	3	1	1,09	56	18	2,4	50	3	0,5	2,16
17	26	1,3	40	1	0,5	1,42	57	18	2,8	70	1	0,5	2,89
18	26	0,8	70	2	1,5	1,33	58	18	2,8	70	2	0,5	2,96
19	26	0,8	70	3	0,5	3,46	59	18	2,8	50	3	0,5	2,28
20	26	0,8	70	3	1,5	1,6	60	18	2,1	70	1	0,5	3,01
21	26	0,8	60	1	1	1,64	61	18	2,1	70	1	1	1,79
22	26	0,8	60	2	0,5	3,07	62	18	2,1	70	2	0,5	3,1
23	26	0,8	60	2	1	1,99	63	18	2,1	60	2	0,5	2,42
24	26	0,8	60	3	0,5	3,15	64	18	2,1	50	2	0,5	2,13
25	26	0,8	50	2	1	1,02	65	24	1,1	70	1	0,5	3,12
26	26	2,4	70	1	1	2,2	66	24	1,1	70	3	1	2,83
27	26	2,4	70	2	0,5	2,81	67	24	1,1	60	1	0,5	2,19
28	26	2,4	60	3	0,5	2,41	68	24	1,1	60	2	0,5	2,23
29	26	2,4	50	1	0,5	1,96	69	24	1,1	50	1	0,5	1,87
30	26	2,4	50	3	0,5	2,06	70	24	1,3	70	2	0,5	3,32
31	26	2,4	40	3	0,5	1,15	71	24	1,3	70	2	1	2,19
32	26	2,8	70	1	0,5	3,09	72	24	1,3	70	3	1	2,23
33	26	2,8	70	1	1	2,06	73	24	1,3	60	1	0,5	2,76
34	26	2,8	70	2	1	2,16	74	24	1,3	50	2	0,5	2,41
35	26	2,8	50	1	0,5	1,87	75	24	0,8	70	1	0,5	3,25
36	26	2,8	40	1	0,5	1,14	76	24	0,8	70	2	0,5	3,34
37	26	2,1	70	2	0,5	3,21	77	24	2,4	70	1	0,5	3,04
38	26	2,1	70	3	0,5	3,26	78	24	2,4	50	2	0,5	2,39
39	26	2,1	60	2	1	1,59	79	24	2,4	50	3	0,5	2,43
40	18	1,1	70	1	0,5	2,92	80	24	2,8	70	1	0,5	3,11
Validation set													
81	26	1,1	50	2	0,5	2,47	101	26	2,1	60	3	1	1,62
82	26	1,1	50	3	0,5	2,73	102	26	2,1	60	3	1,5	1,01
83	26	1,3	60	2	0,5	2,81	103	26	2,1	50	1	0,5	2,01
84	26	1,3	60	2	1	1,61	104	26	2,1	50	2	0,5	2,11
85	26	1,3	50	3	0,5	2,24	105	26	2,1	40	3	0,5	1,14
86	26	0,8	70	3	1	2,92	106	18	1,1	70	1	1	1,63
87	26	0,8	50	3	0,5	2,8	107	18	1,1	70	2	0,5	3,02
88	26	2,4	70	1	0,5	2,73	108	18	1,1	70	2	1	1,87
89	26	2,4	70	2	1	2,31	109	18	1,1	50	1	0,5	1,6
90	26	2,4	70	3	0,5	2,88	110	18	1,1	50	3	0,5	1,73
91	26	2,4	60	3	1	1,58	111	18	0,8	60	2	0,5	2,58
92	26	2,4	50	2	0,5	2,01	112	18	0,8	60	2	1	1,27
93	26	2,8	70	2	0,5	3,14	113	18	2,4	70	3	0,5	3,23
94	26	2,8	60	3	1	1,37	114	18	2,1	50	3	0,5	2,16
95	26	2,8	50	2	0,5	1,91	115	24	1,3	70	3	0,5	3,39
96	26	2,8	50	3	0,5	1,96	116	24	1,3	50	3	0,5	2,43
97	26	2,1	70	1	1,5	1,01	117	24	0,8	50	2	0,5	2,61
98	26	2,1	70	2	1	2,12	118	24	0,8	50	3	0,5	2,69
99	26	2,1	70	3	1	2,15	119	24	2,4	60	3	0,5	2,81
100	26	2,1	60	3	0,5	3,09	120	24	2,8	70	2	0,5	3,21

3.2. Principal Component Analysis (PCA) Result

The table 2 presents factorial weights of variables PCA. The cumulative variances of the three factors are 68.2%. This percentage is close to 70% so most of the information is expressed. The factor 1 is strongly and positively correlated to the concentration of BHT in *attiéké*. Concerning factor 2, it is positively correlated to the packaging temperature (T) and to depth of *attiéké* ball (P). About factor 3, it is negatively correlated to the packaging duration (D).

Table 2. Variances and Factor weights of PCA variables.

	Fact. 1	Fact. 2	Fact. 3
% Variance	28,49	22,34	17,49
Cumulative variance	28,489	50,83	68,32
Variables factor weigh			
C _{BHTsachet}	-0,425	0,025	-0,321
T _{grain}	0,069	-0,264	0,388
T	0,474	0,848	0,017
D	-0,226	-0,079	-0,823
P	-0,650	0,733	0,084
C _{BHTattiéké}	0,909	0,094	-0,333

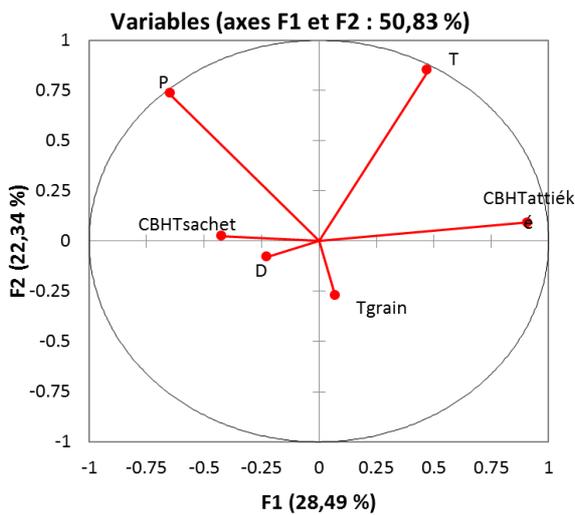


Figure 1. Projection of variables in factorial plane F₁ X F₂.

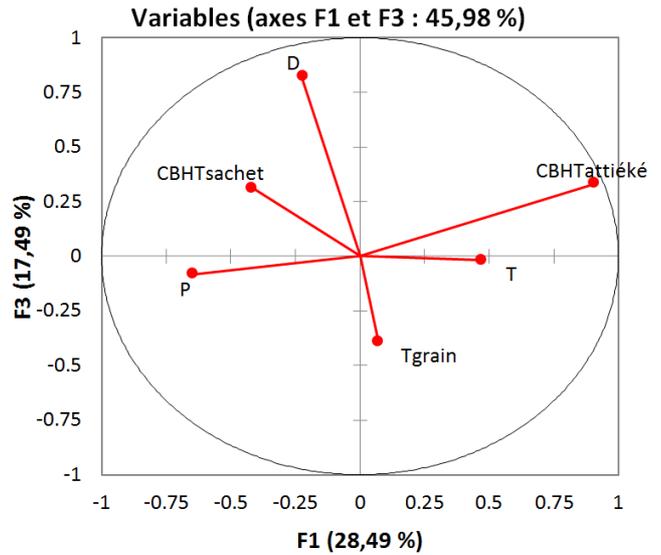


Figure 2. Projection of variables in factorial plane F₁ X F₃.

The figure 1 shows variables projection in the factorial plane F₁ X F₂. This plan shows that the concentration of BHT in *attiéké* (C_{BHTattiéké}) is inversely proportional to the depth level of the *attiéké* ball. As for the F₂ factor, its analysis shows that the temperature and depth level of *attiéké* ball change proportionally. The factorial plane F₁ X F₃ shown in figure 2 indicates that the factor F₃ is negatively correlated to packaging duration. Concerning grain size, it is positively correlated to the same factor. In short, temperature, depth level, grain size and packading duration are involved factors in the transfer of pollutants into the *attiéké*.

3.3. Multiple Linear Regression

Figure 3 shows the linear regression line between the experimental and theoretical values of BHT concentrations in the *attiéké* of the test and validation sets. The point cloud follows practically a straight line of equation $y=0.92x+0.19$.

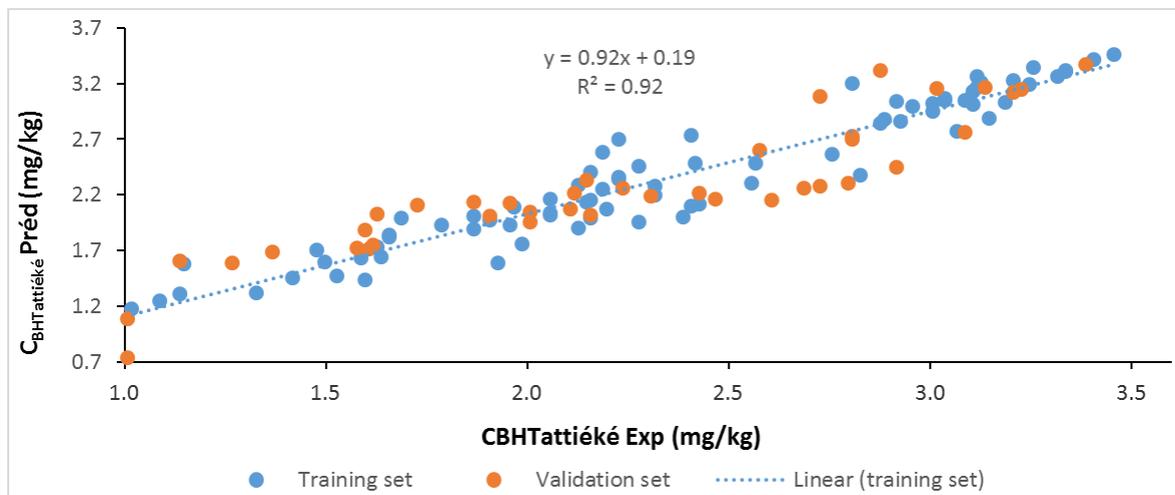


Figure 3. Multiple Linear Regression Line with Test and Validation Sets.

The statistical indicators of the established model are:

$$N = 80; R^2 = 0.92; R^2_{adj.} = 0.915; Q^2_{CV} = 0.913; RMCE = 0.191; F = 170.250$$

3.4. Model Equation

The equation of the multiple linear regression model expressing the concentration of BHT ($C_{BHTattiéké}$) as a function of the different parameters is given below:

$$C_{BHTattiéké} = -0.40135 + 0.02118C_{BHTsachet} - 0.09175T_{grain} + 0.05785T + 0.11435D - 2.02658P$$

In this equation, a positive coefficient indicates that the

BHT concentration evolves in the same direction as the descriptor. However, a negative coefficient indicates that the BHT concentration is inversely proportional to the descriptor.

3.5. Model Validation

Acceptance of the established model is defined as follows:

With $Q^2_{CV} = 0.913$, the model is excellent. $|R^2 - Q^2_{CV}| = 0.007 < 0.3$, the model is predictive.

Fischer test gives a high value $F = 170.250$; which implies that this model is significant. Figure 4 shows the similarity curves between the theoretical and experimental values. Both curves look almost the same.

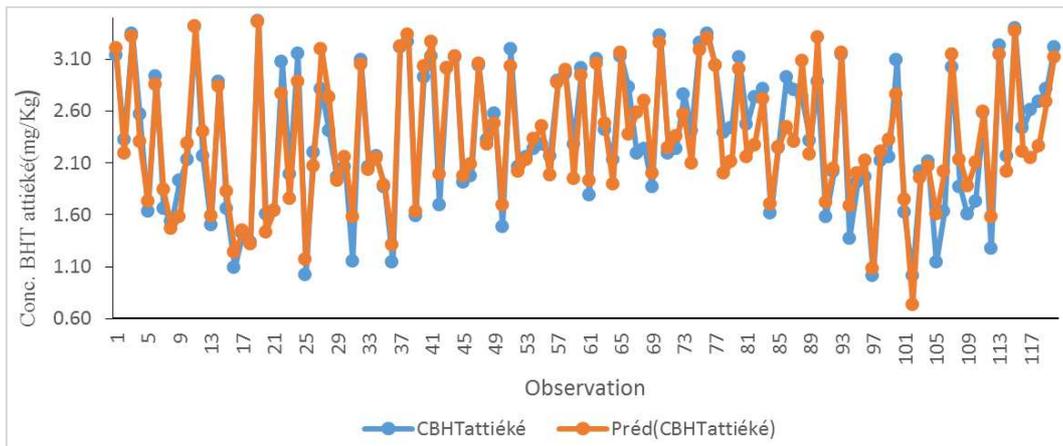


Figure 4. Similarity curve of the MLR model.

In Table 3, the theoretical and experimental concentrations of BHT in *attiéké* were recorded for observations of validation set. The relationships between these two quantities are almost all close to the unit.

Table 3. Relationship between theoretical and experimental concentrations of BHT in *attiéké*.

Observation	$C_{BHTattiéké}$ (mg/Kg) exp	$C_{BHTattiéké}$ (mg/Kg) théo	Cthéo/Cexp	Observation	$C_{BHTattiéké}$ (mg/Kg) exp	$C_{BHTattiéké}$ (mg/Kg) théo	Cthéo/Cexp
81	2,470	2,157	0,870	101	1,620	1,745	1,080
82	2,730	2,271	0,830	102	1,010	0,731	0,720
83	2,810	2,717	0,970	103	2,010	1,951	0,970
84	1,610	1,704	1,060	104	2,110	2,065	0,980
85	2,240	2,253	1,010	105	1,140	1,601	1,400
86	2,920	2,442	0,840	106	1,630	2,017	1,240
87	2,800	2,299	0,820	107	3,020	3,144	1,040
88	2,730	3,080	1,130	108	1,870	2,131	1,140
89	2,310	2,181	0,940	109	1,600	1,873	1,170
90	2,880	3,309	1,150	110	1,730	2,102	1,210
91	1,580	1,717	1,090	111	2,580	2,593	1,010
92	2,010	2,037	1,010	112	1,270	1,580	1,240
93	3,140	3,158	1,010	113	3,230	3,139	0,970
94	1,370	1,680	1,230	114	2,160	2,010	0,930
95	1,910	2,001	1,050	115	3,390	3,367	0,990
96	1,960	2,115	1,080	116	2,430	2,210	0,910
97	1,010	1,081	1,070	117	2,610	2,142	0,820
98	2,120	2,209	1,040	118	2,690	2,256	0,840
99	2,150	2,323	1,080	119	2,810	2,688	0,960
100	3,090	2,758	0,890	120	3,210	3,115	0,970

3.6. Analysis of the Contribution of Descriptors

Figure 5 shows the descriptors that were considered in the

model equation. From this figure, a classification of the most influential descriptors with their respective standardized coefficients was identified. It is the temperature T (0.846) followed by the depth level (from the surface to inside *attiéké*

ball) P (-0.822). In addition, the concentration of BHT is proportional to the temperature, the packaging duration and the initial concentration of BHT in the plastic bag. However,

it is inversely proportional to the grain size of the *attiéké* and the depth of the ball.

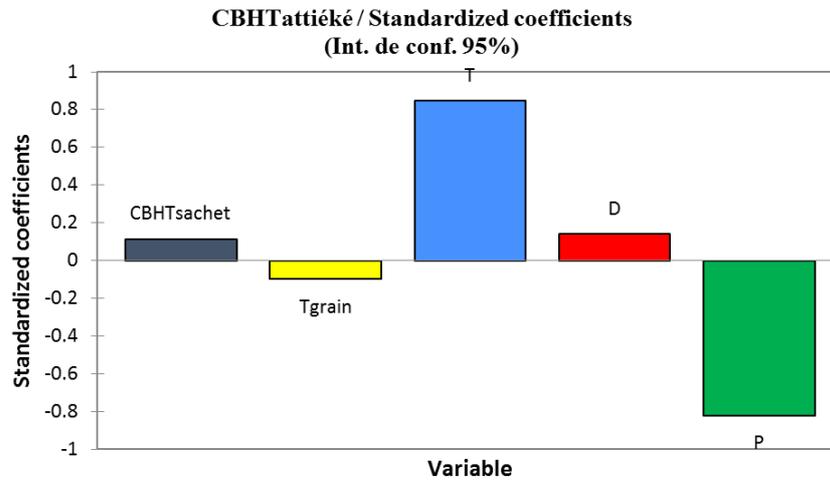


Figure 5. Contribution of physico-chemical descriptors in the model.

4. Discussion

Five (5) descriptors were taken into account in the established model. This number is in accordance with the empirical rule which stipulates that the number of descriptors should be less than or equal to about one-fifth of the number of observations in the learning set [15, 16]. The concentration of BHT in the *attiéké* evolves in the same direction as the temperature, duration and initial concentration of the pollutant in the plastic bag. However, it is inversely proportional to the grain size of the *attiéké* and its level of depth (from surface to inside *attiéké* ball). In addition, temperature is the most important descriptor.

Thus, the increase in temperature considerably favours the migration of pollutants. Musoke *et al.* and Traistaru *et al.* reached the same conclusion [10, 9]. Gao *et al.* detected the migration of BHT from plastic packaging into an aqueous simulant at a temperature of 40°C for a contact time of 10 days [23]. The second most important descriptor is the depth level (from the surface to the inside of the *attiéké* ball). The contact between the packaging and the food is made on the surface, which explains why the contents are higher on the surface than at depth. When the grain size is large, contaminants are more difficult to spread at depth. This observation is in agreement with Sakr *et al.* [24]. According to these authors, grain size affects the adsorption capacity of compounds. The finer the grain size, the greater the specific surface area and the greater the adsorption. According to Sauvegrain, the level of contamination of the food depends on the chemical nature of the substances, the initial amount contained in the materials, the contact surface, the nature of the contact between the materials and the food, the contact duration and the temperature [25]. The ratios of the theoretical and experimental concentrations of the validation set show that this ratio is approximately equal to one (1). This indicates that the model is acceptable. This statement is

confirmed by the similarity curve between the experimental concentrations of BHT in *attiéké* and the theoretical concentrations. The value of the Fischer test being high $F=170.2497$, it implies that the model determined is significant. Temperature, BHT concentration in plastic bag, grain size, depth level and duration provide a significant amount of information to the model [26].

The cross-validation coefficient Q_{CV}^2 is 0.9134; this coefficient being greater than 0.9 then the proposed model is excellent [22].

$R^2-R^2_{adj.}=0.005$, This difference being less than 0.3, it can be said that descriptors choice is acceptable. The difference between Q^2 and R^2 is 0.0066 and therefore less than 0.3. The model is then predictive. It can be used to predict the concentration of BHT in *attiéké* [21]. It should be noted that the model was based on 120 observations; this is a significant number enough to validate the model. This model can be applied for *attiéké* conditioning temperatures ranging from 40 to 70°C and for depth levels varying from the surface to 1.5 cm inside the *attiéké* ball. For conditioning temperatures between 60 and 70°C, BHT concentrations in the *attiéké* are sometimes higher than the specific migration limit set by the European Union Regulation EC n°10/2011 (3 mg/L) in the surface layer (up to 0.5 cm deep) [5].

5. Conclusion

The migration of the antioxidant BHT was modelled using the multiple linear regression method. This method was validated by various statistical indices. The determination coefficient was $R^2=0.92$, the standard deviation was $RMSE=0.1909 < 0.3$. The Fischer test was $F=170.2497$. $Q_{CV}^2=0.9134 > 0.9$, the proposed model is excellent.

$R^2-R^2_{adj.}=0.0054 < 0.3$, then the choice of descriptors is acceptable. $Q_{CV}^2-R^2=0.0066 < 0.3$, so the model is predictive. It can be used to predict the concentration of BHT in *attiéké*. All its indicators confirm that the model determined is

excellent. This study shows that the migration of additives can be limited by the control of the conditioning temperature, which is the most important descriptor. In addition, this migration is low in depth (inside the *attiéké* ball) which represents the second most important descriptor here. To comply with the specific migration limit recommended by the European Union regulation, producers should condition *attiéké* at ambient temperature and consumers should remove the top layer (up to 0.5 cm). This would limit the health risk associated with the consumption of this staple food in Côte d'Ivoire.

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