



Original article

Modelling thermal characteristics of cocoa butter using a feed-forward artificial neural network based on multilayer perceptronOmid Rostami,^{1,2} Farzad Saberi,^{2,3} Amirreza Mohammadi,^{3,4} Leila Kamalirousta,^{2,3} Cristina M. Rosell^{5,6}  & Nicola Gasparre^{5*} 

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Summary

Cocoa butter is the most important ingredient of chocolate, which determines its melting behaviour. Variations in the melting characteristics of cocoa butter can profoundly affect the performance and suitability for their industrial utilisation. Over time, researchers have been attempting to establish a logical relationship between cocoa butter's unique thermal properties and the amount of saturated to unsaturated fatty acids in mono, di and triglycerides, and fatty acids (as major components), and free fatty acids, soap, primary oxidation products, minerals, moisture, phospholipids, tocopherols, unsaponifiable matters and metals (as minor components) found in cocoa butter. In this research, the thermal behaviours of thirteen samples of cocoa butter with different origins were investigated using isothermal differential scanning calorimetry. The cocoa butters starting temperature of crystallisation, temperature of maximum heat release, temperature of completed crystallisation and the enthalpy of heat release during recrystallisation were evaluated. In addition, the chemical composition (moisture, acidity, peroxide, minerals and soap content), fatty acid and triacylglycerol composition were used to establish an MLP-ANN with fourteen input neurons connected by two flexible, sigmoid activation function layers. The back-propagation was used to train the artificial neural network (ANN) structure and optimise the error of prediction. The study showed that the MLP algorithm can predict the thermal behaviour of CB samples with trace error, regardless of plant growth and extract process condition.

Keywords Cocoa butter, DSC, multilayer perceptron, sigmoid activation function.

Introduction

Cocoa butter (CB) is the most important vegetable fat, which is extracted from cocoa beans. CB is the most valuable raw material in chocolate due to its structural (rheological and textural) and chemical characteristics as well as organoleptic qualities (Ewens *et al.*, 2021; Samanta *et al.*, 2022). These characteristics of CB make it suitable for manufacturing various confectionery products. However, the correlation between its major (saturated to unsaturated fatty acids in mono, di, and

triglycerides and fatty acids) and minor components (free fatty acids, soap, primary oxidation products, minerals, moisture, phospholipids, tocopherols, unsaponifiable matters and metals) poses a significant challenge in fully understand their combined impact on the thermal behaviour of CB. Conversely, these components define the thermal aspect of CB, a characteristic influenced by the specific growth conditions of the cocoa tree (Torres-Moreno *et al.*, 2015). Indeed, it is important to note that FFA is closely related to bean diseases and postharvest hydrolysis. Consequently, the FFA content can be also used as a marker for assessing the deterioration quality of the beans beside that they can influence

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the thermal behaviour of the CB (Ostrowska-Ligeza *et al.*, 2021; Houphouet *et al.*, 2023).

Due to this, in recent years, research efforts have been spent to establish a mathematical function that describes the thermal behaviour of CB. Developing such a function poses a challenge since the variable parameters exhibit varying degrees of influence on the final crystallisation behaviour. Previous studies have focused on different aspects, such as the ratio of saturated to unsaturated fatty acids in mono, di, and triglycerides structure, fatty acid composition, free fatty acids, soap content, primary oxidation products, minerals, moisture content, phospholipids, tocopherols, unsaponifiable matter and metals as influential factors of melting and crystallisation behaviour of CB, individually (Fernandes *et al.*, 2013; Wang & Maleky, 2018). These investigations have provided valuable insights into the intricate nature of CB's thermal properties. Building upon this foundational knowledge, advanced computational techniques such as the artificial neural networks (ANN) have emerged as powerful tools in food technology research. With their ability to reduce cost and time, adapt to changing conditions, and operate at high speeds, ANNs is an accurate tool with a crucial role in solving complex problems, especially in food technology, enabling researchers to gain deeper understanding and make accurate predictions (Bhagya Raj & Dash, 2022; Thapa *et al.*, 2023). This mathematical function, drawing inspiration from the human biological neural system, demonstrates remarkable efficacy where conventional statistical methods cannot elucidate the connection between input and output data (Ferrero Bermejo *et al.*, 2019). In the biological system, when the dendrites of a neuron receive ample stimulation at the synaptic joints and the cumulative signal surpasses a critical threshold, they initiate the transmission of an electrochemical signal from the dendrites to the axons, thus, to conveying an electrochemical message (Huang *et al.*, 2007; Baykal & Yildirim, 2013). This system becomes more efficient when receiving messages from multiple nodes and sending them to the surrounding neurons. Technically, ANN models are arranged to find input weight (strength) and mimic synaptic mechanism (eqn 1). Meanwhile, different activation functions are used to determine the threshold limit of each ANN neuron, such as the sigmoid function. This threshold limit is established during the learning period to determine the correct output value (Baykal & Yildirim, 2013).

$$\text{Net} = \sum_{i=1}^n W_{ji} X_i + \text{bias}_j \quad (1)$$

In the net function, the X_1, X_2, \dots, X_n is inputs and W_1, W_2, \dots, W_n is respective weights and noise is added as bias.

In recent years, novel researchers have tried to introduce practical applications for Multilayer Perceptron (MLP)-ANN models specifically when it comes to the effect of parameters, which could not be easily related to each other or to check their whole impact on the features of final matrices. Having input the outcomes from any experiment, which are classified using these specific models, training of the algorithm could be conducted to predict some specific characteristics by spending training periods with the attained results (Ostrowska-Ligeza *et al.*, 2021).

Machine learning has been instrumental in measuring parameters such as toxin levels in foods (Wu *et al.*, 2018), detecting cracked eggshells Deng *et al.* (2010), and analysing food colour (Minz *et al.*, 2020). Furthermore, the application of the ANN has demonstrated promising results, particularly in predicting the meat-ball deep-fat frying process (Mittal & Zhang, 2001) and the shelf life of two varieties of packaged rice snacks (Siripatrawan & Jantawat, 2009) as well as assessing rice milling quality (Zareiforush *et al.*, 2015).

The current study aimed to establish a Feed-Forward Artificial Neural Network based on Multilayer Perceptron to predict the crystallisation behaviour of CB using the determination of different inputs and evaluating the differential scanning calorimetry (DSC) of the CB samples.

Material and methods

Raw material

A selection of thirteen cocoa butter samples was prepared, having different production dates, which were coded as CB1 (Cargill, USA, Ivory Coast origin), CB2, CB3, CB4 (Olam, Netherland, Ghanaian origin), CB5 (Golden Harvest, Indonesia, Indonesian origin), CB6 (Favorich, Malaysia, Malaysian origin), CB7 (Cocoa life, Dominican Republic, Dominican Republic origin), CB8 (Cargill, USA, Ecuadorian origin), CB9, CB10, CB11, CB12, CB13, and (Unknown samples).

Qualitative characteristics

All analysis of CB samples was performed following the AOAC standard methods, including moisture content (method No. 926.08, 1995), acidity (method No. 920.124, 1995), minerals (method No. 960.29, 1995) and AOCS standard methods for peroxide (CD 8-53, 1997), FFA (method Ca 5a-40, 1997) and soap content (method Cc 17-95, 1997).

Fatty acids quantification

The quantification of fatty acids was carried out using gas chromatography (GC) and samples were prepared

following the method described by Samaniego *et al.* (2021) with minor adjustments. Briefly, 50 mg of CB was boiled in a volumetric flask with 2 mL of sodium methoxide and dissolved in methanol (0.2 mol L^{-1}) for 15 min. Following this, a mixture comprising sulfuric acid (dissolved in methanol), 4 mL sodium chloride and 1 mL of isooctane (2,2,4 trimethylpentane) was added.

To find out the amount of the fatty acid composition of each CB sample, a gas chromatograph (GC-2014, Kyoto, Shimadzu, Japan) equipped with a FID detector and a Polar capillary column (Agilent J&W, Santa Clara, CA, USA) measuring 100 m in length was employed. The column was coated with $0.2 \mu\text{m}$ of CP-Sil 88 with an internal diameter of 0.25 mm and a film thickness of 0.2 mm . Hydrogen with a purity of 99.99% was used as carrier gas. Then, $1 \mu\text{L}$ top phase of the supernatant solution was injected into the GC. During the operation, the temperature of the injector and the detector was kept constant at $240 \text{ }^\circ\text{C}$, while the temperature of column oven increased from 120 to $240 \text{ }^\circ\text{C}$ at a rate of $4 \text{ }^\circ\text{C per min}$, and then kept constant at $240 \text{ }^\circ\text{C}$ for 7 min. In order to recognise the peaks in the samples, the obtained retention times were compared against certified reference standards of Fatty Acid Methyl Esters (FAMES) known as Standard 47885-U. These standards were acquired from Sigma-Aldrich (St. Louis, MO, USA). Then, the amount of each fatty acid was determined by dividing the peak area, corresponding to that particular fatty acid by the peak area of all the fatty acids combined (ISO, 12966-4).

Thermal properties

The thermal profile of the CB samples was performed in triplicate through the differential scanning

calorimeter (DSC) (Setaram131, Geneva, Austria). Indium and n-dodecane (Sigma Aldrich) were used for calibration, while an empty pan was used as the reference of the tempering profile. Then, the CB samples (15 mg) were sealed in aluminium pans. During the test, the tempering profile test was set at $60 \text{ }^\circ\text{C}$ for 15 min to destroy all crystal forms. Subsequently, temperature was reduced at a rate of $2 \text{ }^\circ\text{C min}^{-1}$ until it reached $15 \text{ }^\circ\text{C}$ to allow the formation of all possible crystal structures (Colella *et al.*, 2023). The sigmoid model described by Foubert *et al.* (2004) was applied on the DSC graph to calculate the start and the end of crystallisation process. Then, the amount of heat release at the end of the crystallisation was determined using an algorithm developed in MATLAB 2021 software, designed to calculate the area under the curve.

Triacylglycerol profile analysis

The triacylglycerol (TAG) profiles of different samples of chocolates were analysed using high performance liquid chromatography (Agilent HPLC, Santa Clara, CA, USA) equipped with Column ZORBAX C-18 ($4.6 \times 250 \text{ mm}$, $5 \mu\text{m}$, Agilent Technologies) according to the AOCS Official Method Ce 5b-89 (Watanabe *et al.*, 2021).

Artificial neural network methodology

Figure 1 provides a detailed overview of the process involved in developing and selecting the most suitable neural network model for the given prediction task. Utilising MATLAB 2021 software, an MLP model was created. This latter comprised fourteen neurons in the first layer (as row of input data), corresponding to the row of input data, with the configuration of hidden layer of neurons, specified in Table 1. To assess the

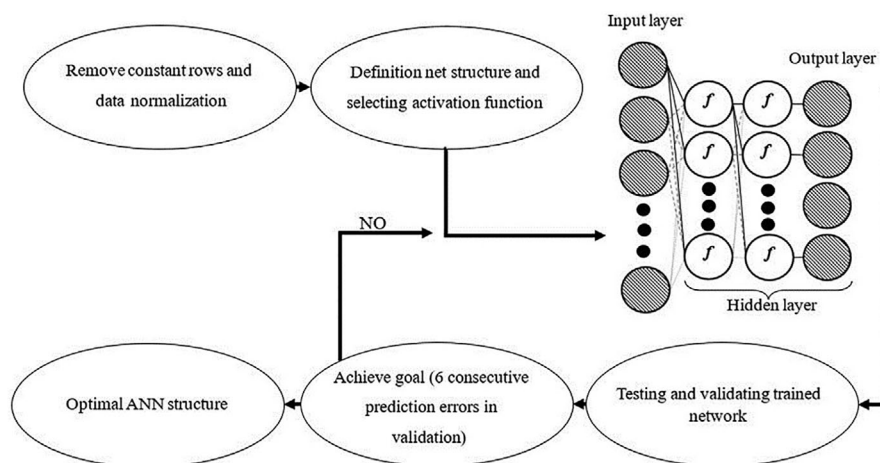


Fig. 1 Schematic diagram of raw data preparation and MLP models.

Table 1 The chemical, fatty acid composition and thermal parameters of cocoa butter samples (CBs)

Sample	Chemical composition					Fatty acid composition					Triacylglycerol composition					DSC		ΔH_f $T_g, ^\circ\text{C}$	ΔH_f J g^{-1}
	Mo, % W/W	Ac, % W/W	Pe, meq kg^{-1}	Mi, mg per 100 g	So, ppm	Palmitic acid, %	Stearic acid, %	Oleic acid, %	Linoleic acid, %	Arachidic acid, %	POP	POS	PLS	SOS	$T_g, ^\circ\text{C}$	$T_{\text{max}}, ^\circ\text{C}$			
CB ₁	0.06 ^{ab}	1.19 ^a	2.2 ^a	0 ^c	558 ^d	27.77 ^b	34.27 ^d	34.53 ^b	2.68 ^b	1.10 ^a	14.9 ^{ba}	37.1 ^c	3.0 ^b	27.8 ^d	34.47 ^d	28.41 ^d	19.13 ^f	8.70 ^a	
CB ₂	0.07 ^a	1.23 ^a	0.33 ^f	0.1 ^{bc}	728 ^b	28.28 ^a	35.20 ^{bc}	33.51 ^c	2.31 ^b	1.09 ^a	15.4 ^a	37.3 ^c	2.6 ^b	28.6 ^c	34.70 ^{cd}	28.74 ^{cd}	19.77 ^e	9.06 ^a	
CB ₃	0.06 ^{ab}	1.07 ^b	1.33 ^b	0 ^c	438 ^e	26.64 ^{de}	34.89 ^c	35.04 ^b	2.94 ^b	0.98 ^{bc}	14.7 ^{bc}	37.6 ^c	3.4 ^a	28.1 ^c	35.72 ^b	29.59 ^b	21.36 ^c	6.35 ^f	
CB ₄	0.07 ^a	0.78 ^{cd}	0.12 ^h	0.3 ^a	818 ^a	26.64 ^{de}	36.02 ^a	34.33 ^b	2.46 ^b	1.00 ^b	14.7 ^{bc}	39.6 ^a	2.7 ^b	30.32 ^a	34.68 ^{bd}	28.75 ^c	19.73 ^e	8.32 ^b	
CB ₅	0.05 ^b	0.50 ^e	0.58 ^e	0 ^c	641 ^c	27.05 ^c	35.20 ^{bc}	34.63 ^b	2.61 ^b	1.00 ^b	14.8 ^{bc}	38.7 ^b	2.9 ^b	28.7 ^c	35.47 ^b	29.27 ^c	21.02 ^c	6.97 ^d	
CB ₆	0.03 ^{cd}	1.01 ^b	1.10 ^c	0 ^c	591 ^d	26.23 ^e	35.40 ^b	34.94 ^b	2.83 ^b	1.06 ^a	14.6 ^{bc}	38.3 ^b	3.2 ^{ab}	29.0 ^{bc}	36.41 ^a	30.46 ^a	22.54 ^a	7.76 ^c	
CB ₇	0.03 ^{cd}	0.66 ^d	0.68 ^d	0.1 ^{bc}	699 ^b	27.05 ^{cd}	35.40 ^b	34.33 ^b	2.76 ^b	1.00 ^b	14.8 ^b	38.6 ^b	3.1 ^{ab}	29.1 ^{bc}	35.89 ^b	29.67 ^b	21.72 ^b	6.96 ^{de}	
CB ₈	0.04 ^{bc}	0.24 ^f	0.23 ^g	0.3 ^a	718 ^b	26.33 ^e	36.22 ^a	34.12 ^{bc}	2.45 ^b	1.01 ^b	14.5 ^{bc}	39.5 ^a	2.7 ^b	30.47 ^a	35.10 ^c	29.01 ^c	20.56 ^d	8.84 ^a	
CB ₉	0.06 ^{ab}	0.78 ^c	0.42 ^f	0 ^c	602 ^c	26.84 ^{de}	35.50 ^{ba}	34.43 ^b	2.80 ^b	0.91 ^c	14.7 ^{bc}	39.4 ^a	3.2 ^{ab}	29.3 ^b	36.14 ^a	30.14 ^b	22.12 ^b	7.91 ^b	
CB ₁₀	0.07 ^a	0.12 ^g	0.10 ^h	0 ^c	406 ^e	25.51 ^f	31.71 ^e	38.53 ^a	3.80 ^a	0.95 ^{bc}	14.3 ^c	37.3 ^c	3.7 ^a	26.9 ^b	36.88 ^a	30.78 ^a	22.73 ^a	7.26 ^d	
CB ₁₁	0.05 ^b	0.29 ^f	1.01 ^c	0.2 ^{ab}	810 ^a	27.36 ^{cd}	35.40 ^b	34.22 ^{bc}	2.42 ^b	1.01 ^b	15.1 ^a	38.5 ^b	2.7 ^b	29.1 ^{bc}	35.02 ^c	28.94 ^c	20.27 ^d	6.87 ^e	
CB ₁₂	0.02 ^d	0.17 ^g	1.00 ^c	0 ^c	611 ^c	26.43 ^e	35.81 ^a	34.33 ^b	2.87 ^b	1.09 ^a	14.5 ^{bc}	38.9 ^a	3.6 ^a	29.6 ^b	36.29 ^a	30.36 ^a	22.49 ^a	6.98 ^{de}	
CB ₁₃	0.05 ^b	0.70 ^d	0.52 ^e	0 ^c	702 ^b	26.33 ^e	36.02 ^a	34.53 ^b	2.46 ^b	1.10 ^a	14.4 ^c	39.3 ^a	2.8 ^b	30.34 ^a	34.98 ^c	28.97 ^c	20.34 ^d	6.89 ^e	

All of the standard deviations were less than $\pm 3.5\%$.

Ac, Acidity; Mi, minerals; Mo, moisture; Pe, peroxide; So, soap content; T_g , temperature of end crystallisation; T_{max} , peak temperature; T_g , Start temperature of crystallisation. Means in the same column with different superscript letters indicate significant difference at $P < 0.05$.

validity of the models, statistical parameters such as correlation coefficients were evaluated for the training set (R_{train}), test set (R_{test}) and validation set ($R_{\text{validation}}$).

Statistical analysis

To run the analysis of variance (ANOVA) and the significance mean levels (Duncan) ($P < 0.05$), all the data obtained were processed through the SAS software version 9.2 (SAS Institute, Cary, NC, USA). Additionally, Principal Component Analysis (PCA) was performed using Minitab 18 software (Minitab, LLC, Penn State University) for clustering the results.

Result and discussion

Multilayer perceptron–MLP

The results showed that there is a strong correlation between the composition of CB and its crystallisation behaviour. The composition of the CB samples includes the chemical features, impurities (soap, primary oxidation products, minerals and moisture) as well as the fatty acid and TAG compositions. Table 1 shows the results for the thirteen CB samples arranged in decreasing order of temperature ranging from 60 to 19 °C, to fully solidify the CB oils. The findings indicate significant variations ($P < 0.05$) in the quantities among the samples, leading to different DSC outcomes. Notably, impurities such as soap contributed to lower temperatures for both start and finish the crystallisation process. The same phenomenon occurred when the acidity and peroxide values increased. This observation aligns with the findings from Ayala *et al.* (2007), which reported a reverse-linear correlation between solid fat content and the FFA content of CB. In fact, the crystal-hindering components play a blocking role on the crystal bonding site (Herrera & Marquez Rocha, 1996). Generally, the set point of the crystallisation, which is known as T_c , tends to be lower, necessitating a more significant decrease in temperature to achieve enough fat crystal formation to solidify the CB. Considering that long-chain fatty acids, such as stearic acid, have higher melting points, a higher quantity of stearic acid and consequently, a higher stearic-oleic-stearic content of TAG, would prompt CB to initiate fat crystals formation earlier compared to other types of fatty acids and TAGs. Moreover, based on the results from Table 1, the effect of a lower quantity of impurities and fewer chemical compounds are higher than the effect of higher quantities of stearic acid and SOS. Therefore, the interaction of all the mentioned parameters leads to CB10 and CB1 exhibiting significantly ($P < 0.05$) the highest and the lowest quantities of DSC factors,

respectively. Figure 1 illustrates the schematic diagram of this process, where the first functional layer has two and four neurons followed by four and eight neurons in the second active layer. To predict CB's thermal properties, the data underwent pre-adjustment to remove constant rows and normalised data. A flexible range of neurons in the first and second hidden layers was used to design the MLP algorithms. This study used fourteen input neurons to enter chemical, fatty acid, and triacylglycerol composition into a straight-forward network (one flow of data from input to output), a familiar ANN for pattern recognition. The first layer, serving as the input layer in Fig. 1, does not contain functional neurons but is utilised as a conductor for each variable to reach the hidden layer. The number of nodes in the input layer depends on CB variables, while the concentration of nodes in the hidden layer is determined experimentally without following a standard pattern. One of the most helpful training algorithms for a feed-forward MLP is back propagation (BP), which computes the weight of nodes to minimise prediction error between accurate results and forecasts (Jahani, 2019; Singh *et al.*, 2022). In this study, ANN models were trained by using the BP algorithm, with 70% of the data (ten samples) used for training and the remaining 30% (three samples) for testing. The sigmoidal function determined the threshold for entry data into the following functional nodes. The model's performance was evaluated as an MLP learning indicator, as shown in Table 2. The performance graph indicated a decreasing trend of error in the training process, depicted by the blue colour. However, as the number of functional neurons in hidden layers increased, the validation and test errors of the models also increased. This rise in validation and test errors signify overtraining of the model. Previous research has reported that an enlarged function layer leads to increased error, as the model attempts to fit the data, including natural analysis instrument error (Balkhi & Moallem, 2022; Mohammadzadeh *et al.*, 2022). The optimal MLP model for predicting thermal properties with a favourable learning rate was found to have four neurons in both the first and second functional hidden layers, achieving a model performance of 2.79.

Principal component analysis

To gain a comprehensive understanding of the impact of the different variables of CB on its characteristics, a principal component analysis (PCA) was conducted (Fig. 2). The PCA explained 45.7% and 22.1% of the variability with two components, PC1 and PC2, respectively. Overall, an increase in CB impurities corresponded to a decrease in both the starting and ending temperature of fat crystallisation. However, when

Table 2 The models of functional layers and performance parameter of models

Model	Hidden layers			Performance model	R_{train}	Training correlation	R_{test}	Test correlation	$R_{validation}$	Validation correlation	Performance plot
	IL	FHL	SHL								
1	14	2	4	6.588	0.99		0.96		0.96		
2	14	2	8	3.973	0.99		0.92		0.98		
3	14	4	4	2.790	0.99		0.99		0.99		
4	14	4	8	9.521	0.99		0.96		0.97		

IL, Input layer; FHL, first hidden layer; SHL, second hidden layer.

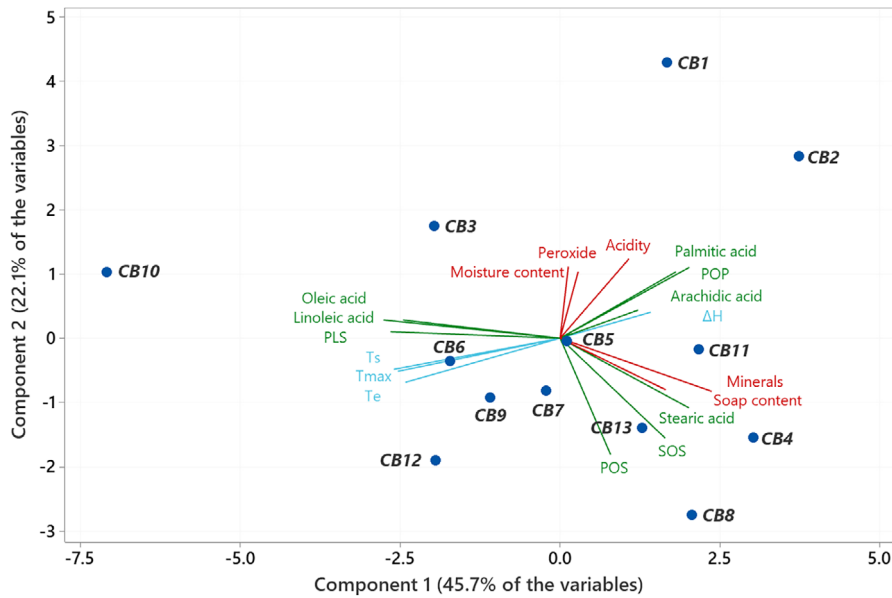


Fig. 2 PCA graph of the effect of different parameters on the crystallisation behaviour.

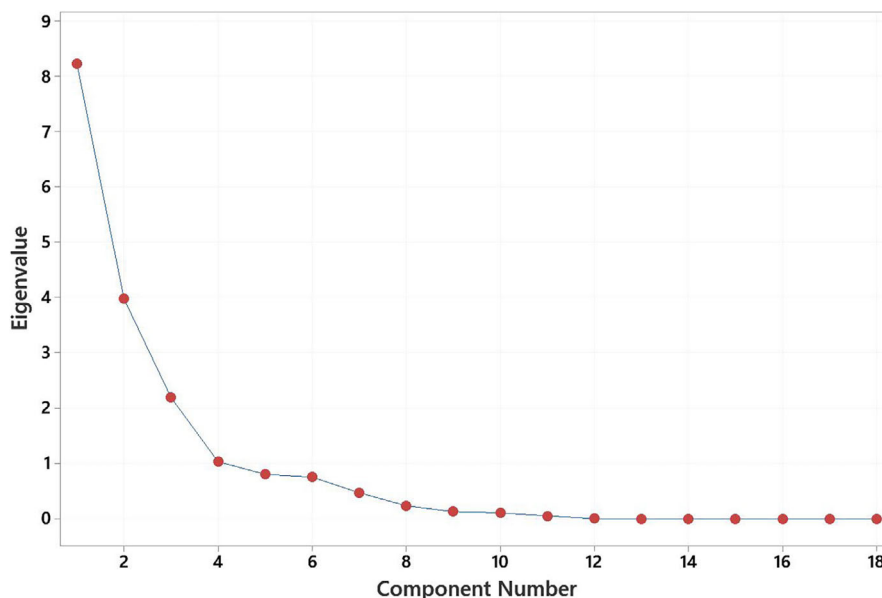


Fig. 3 Scree plot of eigenvalues of different components.

Table 3 Eigenvectors of the chemical, fatty acid composition and thermal parameters of cocoa butter samples

Variables	PC1	PC2	PC3	PC4
Soap content	0.288			
Minerals	0.201			
SOS	0.2			
ΔH	0.172			
POS	0.096			
Acidity		0.31		
Palmitic acid		0.277		
Moisture content		0.26		
Linoleic acid		0.072		
Oleic acid		0.071		
Peroxide			0.436	
Arachidic acid			0.367	
Stearic acid			0.256	
PLS			0.158	
POP				0.495
T_e				0.296
T_s				0.257
T_{max}				0.241

T_e , Temperature of end crystallisation; T_{max} , Peak temperature; T_s , Start temperature of crystallisation.

considering the types of fatty acids and triglycerides, their effects on crystallisation curve was found to be entirely different. In terms of other effective components of PCA, components 3 and 4 (Fig. 3) exhibited eigenvalues higher than 1, accounting for 12.2% and 5.7%, respectively. The cumulative variance explained by the first four components reached 85.7% which

includes the most significant data. According to Table 3, it could be seen that soap content, minerals, SOS, ΔH and POS alongside acidity, palmitic acid, moisture content, linoleic acid and oleic acid contributed to the majority of variances (67.7%). This signifies their pivotal role in shaping the observed variance patterns within the dataset. In particular, CB1 and CB samples (upper right quadrant) showed higher values of acidity, peroxides and palmitic acid and were uniform in terms of enthalpy, arachidic acid and POP. On the other hand, in the upper left quadrant, CB3 and CB10 displayed similar contents of oleic and linoleic acids together with PLS. Comparable results about start, peak and end temperatures of crystallisation were found among the samples located in the lower left quadrant (CB6, CB7, CB9 and CB12), whereas those present in the lower right quadrant (CB4, CB5, CB8, CB11 and CB13) exhibited homogeneous values of stearic acid, POS and SOS.

Conclusion

The outcomes of the study showed that the rate of solidification of CB was highly dependent on its chemical composition, which in turn significantly influences its crystallisation behaviour. One notable aspect of this research lies in its achievement of accurately predicting thermal outcomes through conventional methodologies grounded in widely accepted standards. Owing to that, the developed ANN model, based on MLP, could offer several avenues for implementation in industrial settings. Firstly, by integrating the proposed model into existing

production processes, manufacturers can enhance their ability to predict and control the crystallisation behaviour of cocoa butter. This predictive capability is crucial for ensuring consistent product quality and optimising manufacturing efficiency. The ANN model's ability to handle multiple variables simultaneously enables a holistic approach for process optimisation and troubleshooting, as it could allow manufacturers to identify and address potential bottlenecks or inefficiencies in their production workflows. For instance, this model could be key in the optimisation of tempering processes, which is a critical step in chocolate production, where controlled crystallisation of cocoa butter is essential for achieving desired texture, gloss and snap in the final product. By inputting relevant parameters such as fatty acid composition, impurity levels and thermal properties into the trained ANN model, manufacturers can obtain accurate predictions of the crystallisation behaviour of cocoa butter samples under varying conditions. These predictions can then inform decisions regarding tempering temperature profiles, cooling rates and agitation techniques, ultimately leading to improved process efficiency and product quality. Furthermore, the ANN model can assist in quality control measures by providing early detection of deviations in crystallisation behaviour. Through real-time monitoring of key parameters and comparison with the predictions generated by the ANN model, manufacturers can identify potential issues before they escalate, allowing for timely adjustments to production processes. This proactive approach to quality control can help minimise product defects, reduce waste and enhance overall operational efficiency.

Conflict of interest

The authors declare no conflicts of interest.

Author contributions

Omid Rostami: Writing – original draft; formal analysis; methodology; conceptualization. **Farzad Saberi:** Conceptualization; writing – original draft; methodology; writing – review and editing; formal analysis; data curation. **Amirreza Mohammadi:** Writing – original draft; methodology; formal analysis; writing – review and editing; investigation; visualization. **Cristina M. Rosell:** Writing – review and editing; supervision. **Nicola Gasparre:** Writing – review and editing; writing – original draft; supervision. **Leila Kamalirousta:** Writing – review and editing; validation.

Peer review

The peer review history for this article is available at <https://www.webofscience.com/api/gateway/wos/peer-review/10.1111/ijfs.17298>.

Data availability statement

The data that support the findings of this study are available on request from the corresponding author.

Ethical approval

Ethics approval was not required for this research.

References

- AOAC (1995). *Official Methods of Analysis*, 16th edn. Washington, DC: Association of Official Analytical Chemists.
- AOCS (1997). *Official methods and recommended practices of American Oil Chemists' Society*, 4th edn. Champaign: American Oil Chemists' Society Press.
- Ayala, J.V., Calliauw, G., Foubert, I., Dewettinck, K., Dyer, B. & Greyt, W.D. (2007). Impacts of bleaching and packed column steam refining on cocoa butter properties. *Journal of the American Oil Chemists' Society*, **84**, 1069–1077. This article gives valuable insights into how specific processing techniques can impact the final properties of cocoa butter, which is essential for our research on cocoa butter crystallisation behaviour. We cited this paper to reinforce the importance of considering the effects of factors such as soap, acidity and peroxide values on the crystallisation process, given that our observations aligned with the findings of the cited paper.
- Balkhi, P. & Moallem, M. (2022). A multipurpose wearable sensor-based system for weight training. *Automation*, **3**, 132–152.
- Baykal, H. & Yildirim, H.K. (2013). Application of artificial neural networks (ANNs) in wine technology. *Critical Reviews in Food Science and Nutrition*, **53**, 415–421.
- Bhagya Raj, G.V. & Dash, K.K. (2022). Comprehensive study on applications of artificial neural network in food process modeling. *Critical Reviews in Food Science and Nutrition*, **62**, 2756–2783. This paper provides a comprehensive review of the applications of artificial neural networks (ANNs) in food process modelling. It discusses various aspects of ANNs, including their use in predicting food properties and optimising processing conditions. Since our study involves the use of ANNs for predictive modelling, this reference serves as a foundational piece to understand the broader context and applications of ANNs in the food industry.
- Colella, M.F., Marino, N., Oliviero Rossi, C., Seta, L., Caputo, P. & De Luca, G. (2023). Triacylglycerol composition and chemical-physical properties of cocoa butter and its derivatives: NMR, DSC, X-ray, rheological investigation. *International Journal of Molecular Sciences*, **24**, 2090.
- Deng, X., Wang, Q., Chen, H. & Xie, H. (2010). Eggshell crack detection using a wavelet-based support vector machine. *Computers and Electronics in Agriculture*, **70**, 135–143.
- Ewens, H., Metilli, L. & Simone, E. (2021). Analysis of the effect of recent reformulation strategies on the crystallization behaviour of cocoa butter and the structural properties of chocolate. *Current Research in Food Science*, **4**, 105–114.
- Fernandes, V.A., Müller, A.J. & Sandoval, A.J. (2013). Thermal, structural and rheological characteristics of dark chocolate with different compositions. *Journal of Food Engineering*, **116**, 97–108.
- Ferrero Bermejo, J., Gómez Fernández, J.F., Olivencia Polo, F. & Crespo Márquez, A. (2019). A review of the use of artificial neural network models for energy and reliability prediction. A study of the solar PV, hydraulic and wind energy sources. *Applied Sciences*, **9**, 1844.
- Foubert, I., Vanrolleghem, P.A., Thas, O. & Dewettinck, K. (2004). Influence of chemical composition on the isothermal cocoa butter crystallization. *Journal of Food Science*, **69**, E478–E487. This study was cited to understand the influence of chemical composition, particularly fatty acid composition, on cocoa butter crystallisation.

- Given that our research focuses on the prediction of the crystallisation behaviour of cocoa butter, this reference provides pertinent information on how variations in chemical composition can affect it.
- Herrera, M.L. & Marquez Rocha, F.J. (1996). Effects of sucrose ester on the kinetics of polymorphic transition in hydrogenated sunflower oil. *Journal of the American Oil Chemists' Society*, **73**, 321–326.
- Houphouet, K.R., Tape, J.S., Kouassi, K.I. *et al.* (2023). Occurrence of free fatty acids (FFA) in cocoa beans with various main geographical origin of Côte D'ivoire in the climate change context. *Current Journal of Applied Science and Technology*, **42**, 1–11.
- Huang, Y., Kangas, L.J. & Rasco, B.A. (2007). Applications of artificial neural networks (ANNs) in food science. *Critical Reviews in Food Science and Nutrition*, **47**, 113–126.
- Jahani, A. (2019). Forest landscape aesthetic quality model (FLAQM): a comparative study on landscape modelling using regression analysis and artificial neural networks. *Journal of Forest Science*, **65**, 61–69.
- Minz, P.S., Sawhney, I.K. & Saini, C.S. (2020). Algorithm for processing high definition images for food colourimetry. *Measurement*, **158**, 107670.
- Mittal, G.S. & Zhang, J. (2001). Artificial neural network for the prediction of temperature, moisture and fat contents in meatballs during deep-fat frying. *International Journal of Food Science & Technology*, **36**, 489–497. This paper was referenced to illustrate the application of the ANNs in predicting food properties during thermal processing. Although not directly related to chocolate production, this study demonstrates the versatility of ANNs in predicting temperature, moisture and fat contents during food frying processes. Our research involves predicting thermal properties in chocolate processing, and this reference showcases the potential of ANNs in similar food processing contexts.
- Mohammadzadeh, A., Sabzalian, M.H., Castillo, O., Sakthivel, R., El-Sousy, F.F. & Mobayen, S. (2022). Multilayer perceptron (MLP) neural networks. In: *Neural Networks and Learning Algorithms in MATLAB*. Pp. 5–21. Cham: Springer International Publishing.
- Ostrowska-Ligeza, E., Dolatowska-Zebrowska, K., Wirkowska-Wojdyła, M., Bryś, J. & Górska, A. (2021). Comparison of thermal characteristics and fatty acids composition in raw and roasted cocoa beans from Peru (criollo) and Ecuador (Forastero). *Applied Sciences*, **11**, 2698.
- Samaniego, I., Espín, S., Quiroz, J. *et al.* (2021). Effect of the growing area on the fat content and the fatty acid composition of Ecuadorian cocoa beans. *International Journal of Food Sciences and Nutrition*, **72**, 901–911. This study offers a thorough evaluation of cocoa fat composition across different origins, providing valuable insights into how environmental factors and geographical origin affect the composition of cocoa beans. It was included to better understand the heterogeneity of the fatty acids and to have the whole picture of the fat profile of cocoa beans.
- Samanta, S., Sarkar, T., Chakraborty, R. *et al.* (2022). Dark chocolate: an overview of its biological activity, processing, and fortification approaches. *Current Research in Food Science*, **5**, 1916–1943.
- Singh, A., Kushwaha, S., Alarfaj, M. & Singh, M. (2022). Comprehensive overview of backpropagation algorithm for digital image denoising. *Electronics*, **11**, 1590.
- Siripatrawan, U. & Jantawat, P. (2009). Artificial neural network approach to simultaneously predict shelf life of two varieties of packaged rice snacks. *International Journal of Food Science & Technology*, **44**, 42–49.
- Thapa, A., Nishad, S., Biswas, D. & Roy, S. (2023). A comprehensive review on artificial intelligence assisted technologies in food industry. *Food Bioscience*, **7**, 103231.
- Torres-Moreno, M., Torrecasana, E., Salas-Salvadó, J. & Blanch, C. (2015). Nutritional composition and fatty acids profile in cocoa beans and chocolates with different geographical origin and processing conditions. *Food Chemistry*, **1**, 125–132.
- Wang, H. & Maleky, F. (2018). Effects of cocoa butter triacylglycerides and minor compounds on oil migration. *Food Research International*, **1**, 213–224.
- Watanabe, S., Yoshikawa, S. & Sato, K. (2021). Formation and properties of dark chocolate prepared using fat mixtures of cocoa butter and symmetric/asymmetric stearic-oleic mixed-acid triacylglycerols: impact of molecular compound crystals. *Food Chemistry*, **339**, 127808.
- Wu, Q., Xie, L. & Xu, H. (2018). Determination of toxigenic fungi and aflatoxins in nuts and dried fruits using imaging and spectroscopic techniques. *Food Chemistry*, **252**, 228–242.
- Zareiforush, H., Minaei, S., Alizadeh, M.R. & Banakar, A. (2015). A hybrid intelligent approach based on computer vision and fuzzy logic for quality measurement of milled rice. *Measurement*, **66**, 26–34.