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Using artificial neural networks in prediction of the drying process of foods that are rich in sugars

Uso de redes neuronales artificiales para predecir el proceso de secado por aspersión de alimentos ricos en azúcares

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Abstract
The production of sugar-rich foods powder (SRF) has great economic potential, however, SRF introduced in the spray drying process (SDP) presents adhesion problems in the dryer that cause low yields due to its low temperature of glass transition (Tg), the means of transport like maltodextrin (Mdx) are used to increase your Tg, but there is not an exact dose for all SRF; this because the SRF are very variable in their Tg due to the composition of their sugars; however, models have been developed to predict the amount of Mdx only for some SRF. Artificial neural networks (ANN) are efficient empirical methods for prediction, especially for nonlinear systems. Therefore, the objective of this work was to develop a mathematical model using ANN backpropagation to predict SDP of SRF and avoid adhesion problems, 6 input variables Mdx, fructose (F), glucose (G), sucrose (S), temperature (T), Organic acids (OA) and 6 outlets, humidity (H), Tg, degrees Brix (°BX), hygroscopicity (HI), water activity (WA) and Yield (R). The predictive model of the sugar-rich food system (PMSSRF) consists of 4 layers 10-16-14-10 neurons, respectively, were compared with experimental data using orthogonal regression and shows that PMSSRF predicts SRF SDP, particularly predicts the required concentration of Mdx and powder quality for SRF.
Keywords: Spray drying, artificial neural networks (ANN), maltodextrin (Mdx), sugar-rich foods (SRF).

Resumen
La producción de polvo alimenticio rico en azúcar (SRF) tiene un gran potencial económico, sin embargo, el SRF introducido en el proceso de secado por aspersión (SDP) presenta problemas de adhesión en el secador que causan bajos rendimientos debido a su baja temperatura de transición vítrea (Tg), los medios de transporte como la maltodextrina (Mdx) se usan para aumentar su Tg, pero no existe una dosis exacta para todos los SRF; esto porque los SRF son muy variables en su Tg debido a la composición de sus azúcares; sin embargo, se han desarrollado modelos para predecir la cantidad de Mdx solo para algunos SRF. Las redes neuronales artificiales (ANN) son métodos empíricos eficientes para la predicción, especialmente para sistemas no lineales. Por lo tanto, el objetivo de este trabajo fue desarrollar un modelo matemático utilizando la propagación inversa ANN para predecir SDP de SRF y evitar problemas de adhesión, se tomaron 6 variables de entrada Mdx, fructosa (F), glucosa (G), sacarosa (S), temperatura (T) , Se tomaron ácidos orgánicos (OA) y 6 de salidas humedad (H), Tg, grados Brix (°BX), higroscopicidad (HI), actividad de agua (WA) y Rendimiento (R). El modelo predictivo del sistema alimentario rico en azúcar (PMSSRF) consta de 4 capas 10-16-14-10 neuronas respectivamente, se comparó con datos experimentales mediante regresión ortogonal y muestra que PMSSRF predice el SDP de los SRF, particularmente predice la concentración requerida de Mdx y calidad de polvo para los SRF.
Palabras clave: Secado por aspersión, redes neuronales artificiales (ANN), maltodextrina (Mdx), alimentos ricos en azúcar (SRF).

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1 Introduction

The production of dehydrated powder starting from SRF for example, fruit juices and mashes, has great economic potential due to low-cost storage and transportation. The preferred technique to obtain the powder of SRF is spray drying, this according to the low time of process and temperatures (> 100 °C) to which is the product is processed (Robaina *et al*., 2019; Ho *et al*., 2019). However, the thermoplastic and hygroscopic properties from SRF bring issues during the drying process. These types of foods are composed of high sugar contents (over 90%) such as S, G, F, and OA, that are known by presenting low molecular weight and Tg oscillates between 5 and 62 °C, which causes that solidly adhere to drying walls (Ho *et al*., 2019; Chong *et al*., 2019). The Tg has been recognized as a fundamental parameter to explain the adherence of amorphous and semi-crystalline foods, particularly in the case of carbohydrates due to their low molecular weight. On the other hand, the stickiness problem is not shown when there are carrier agents, these agents are derived from starch and hydrolyze smoothly in spray drying, like maltodextrin. This type of product facilitates the spray drying process of the SRF and is one of the most used in this process (Bhandari *et al*., 1997, 1999; Kaderides *et al*., 2019; Ho *et al*., 2019; Pandey *et al*., 2019). Many studies have shown that the use of Mdx during the powder production of SRF, through spray drying, increases drying performance about 10 and 30% and reduces the content of humidity (Zhang *et al*., 2019); however, it was not specified, the amount of Mdx for all SRF (Adhikari *et al*., 2003). Bhandari *et al*. (1997), developed a linear semi-empirical model to predict the amount of Mdx (6 dextrose), necessary for spray drying a product rich in sugar based on its composition, they determined the values of the individual drying index of S, G, F, and OA; therefore, the model they obtained was linear. On the other hand, this method requires a considerable amount of testing and the interactive effects between the parameters were not studied and their responses are not fully described (Lisboa *et al*., 2018). In this sense, there are different alternatives to solve the aforementioned, such as multivariate statistical techniques (response surfaces, factorial designs) that are used to optimize the process based on two or more variables (Barabadi *et al*., 2019) and artificial neural network (ANN) is another alternative (Barroso-Maldonado *et al*., 2018; Kumar *et al*., 2018; Przybył *et al*., 2018; Yingngam *et al*., 2018; Ghosh *et al*., 2019; Brusamarello *et al*., 2020). The ANN are mathematical models that allow model the drying processes and that achieve better results than other techniques (Aliakbarian *et al*., 2018; Rahmawati *et al*., 2019). However, these current models are only applicable to fruit juices in specific that went through experimentation; in other words, it does not specify a range of concentration for each type of SRF. In this context, it is probable that the ANN modeling inverse propagation allows predicting optimum values of a powder product such as the R, WA, H, °BX, HI and Tg in the function of the type and sugar concentrations as well as different amounts of Mdx. As previously mentioned, the objective of this work was to develop a mathematical model through ANN backpropagation to predict the spray drying process for all SRF, this model allows to predict the necessary encapsulation ratio (Mdx) for the product have no adhesion problems, just knowing types and concentrations of sugars, it is also able to predict dry product specifications like R, WA, H, °BX, HI and Tg for a pilot-scale spray drying.

2 Materials and methods

2.1 Materials and sample preparation

The system sugar-rich food (SSRF) is generated by food-grade sugars F, G and S from the ADM, Innidigo and ZUCARMEX brands, mixed in 4 proportions: 0, 33, 66 and 100%, concerning one liter of water, citric acid (CA) obtained from the drug store "La Paz", in Guadalajara, Jalisco, Mexico, was used as an equivalent of the OA and was added to the mixture of sugars in 0 and 1%, with respect to the same proportion that the sugars, the mixture were homogenized through stirring with which was simulated the composition of the fruit juice from 11-15 °BX (Horuz *et al*., 2012; Sornsomboonsuk *et al*., 2019), then the ºBX were measured with a digital meter (ATAGO®, model POKET Refractometer PAL-3). After stirring, it was added Mdx (Globe) with the equivalent of 10 dextrose and humidity of 4.17% in proportions of 5, 10 and 15%, then again, the mixes were submitted to shaking for 15 min., after that time, the different combinations of the SSRF with Mdx was ready to be submitted to dry (De Souza Lima and Arlabosse, 2020).

The experimental design was completely random, taking into account that there were three types of sugar (F, G, and S) that were mixed in four different proportions, to which two separate amounts of OA were added, two temperature entry conditions in the process spray drying. Finally, three different amounts of Mdx, giving 84 treatments with four replicates, making a total of 336 experimental units of SSRF.

2.2 *Spray drying of the sample*

The drying process was developed in a pilot-scale spray dryer (NIRO-Production mirror®, Germany). The drying operating conditions were inlet air temperature (T) 180 and 190 ºC and outlet temperature of 80 ºC; 150 ml min-1 feed flow and 26,350 RPM spray rate. Drying was fed with each separate experiment. Once the powder was generated for each SSRF, it was stored in a plastic bag in a glass container away from light for further observation. It is important to mention that the initial weight of the SSRF was recorded before the drying process, as the weight of the dehydrated SSRF until the end of the process, in order to calculate the drying performance by equation (1), the result that was considered as a study variable.

$$R = \frac{PF}{PI} \times 100 \tag{1}$$

where R is the yield of drying expressed in percentage (%); PI is the initial weight of the fructose mix, glucose, saccharose, citric acid, and maltodextrin, or SSRF in grams (g), and PF is the final weight of SSRF in g.

2.3 *Physiochemical properties*

After that, the SSRF powders were determined by the following characteristics or variables of the study, H, WA, HI, and Tg, as it is mentioned below: The H was obtained with the method proposed by the AOAC., (1990), that is about calculating the sample; to which was utilized a balance of humidity (PRECISA®, model HA 300-310, Swiss) to register the initial and final weight (after the calculation), while the calcinate was made in a muffle (TERLAB). The WA was registered with a digital meter (AGUALAB®, model LEER, EE. UU.). The values obtained from the activity may vary from 0 to 1. To get the HI has used the method of Cai and Corke. (2000) and was estimated this index by equation (2). The hygroscopicity index is expressed in g of water absorbed by every 100 g of dry matter:

$$HI = \frac{(PV + PMF) - (PV + PMI)}{24} \tag{2}$$

where HI is the hygroscopicity index in g; PV is the glass weight in g; PMF is the final sample weight in g and PMI is the initial sample weight in g.

The Tg was calculated by equation (3) of Fox, according to Gutierrez *et al*. (2004).

$$Tg = \frac{1}{\left(\frac{W_1}{Tg_1}\right) + \left(\frac{W_2}{Tg_2}\right) + \left(\frac{W_n}{Tg_n}\right)} \tag{3}$$

where Tg_1 belongs to the proportion 1, Tg_2 belongs to the proportion 2 and Tg_n belongs to the proportion n, respectively. This expression assumes that the specific volumes of the components of a binary dissolution are approximate equals. Separately, was made a database with the results of the variables of study of the SSRF, that were mentioned previously.

2.4 *Generation of the model artificial neuronal networks*

The ANN model that was developed to simulate the behavior of the experimental data was one of the types of backpropagation, which was developed in the MATLAB mathematical software (Matlab-$R^2$017a, 2017). The network was fed with the experimental data matrix, which was generated in the spray drying of the experimental units. The patterns used in modeling during training were 60 patterns, this matrix was reduced from the initial one that consisted of 84 patterns due to the decision not to take the patterns in which R results as 0; each pattern was obtained from the average of each treatment with its respective replicates. Each pattern had 12 variables, six inputs, and six outputs. The input or input variables were X1-T, X2-F, X3-G, X4-S, X5-OA, and X6-Mdx; while the outputs were Y1-R, Y2-H, Y3-WA, Y4-HI, Y5-Tg, and Y6-°BX were the output ones. The main characteristic of ANN of the backpropagation (it has two different stages: one, on the network training (search of the expected output) and the other, of the application of the trained network to any input and obtaining the respective output) with the limit of one thousand interaction, log-sigmoid transference function and tangential. The training consisted of three stages: (1) advance of the input training pattern, (2) calculus and propagation backward of the associated error, and (3) adjustment of the weights.

2.4.1 Optimization with ANN

The learning optimization process consists of two steps:
Step 1.- To find the neuronal network that with the output data such as the input ones allow to have the objective values, Inverse Network.
Step 2.-To find the neuronal network that with the input data allow us to obtain the objective values. Once the trained network is obtained the input data are applied optimized to get the optimized objective values (Cevallos. 2004).

The neuronal network is trained with six input values X1, X2, X3, X4, X5 and X6 and six output values Y1, Y2, Y3, Y4, Y5 and Y6. Once the network is trained, the optimized values are applied X1, X2, X3, X4, and Y1 as input variables, the network is simulated and it gives us Y2, Y3, Y4, Y5, Y6 and X6 as output values, that are optimized results. The output of the neuronal network that belongs to the input patterns was compared to the objective values and the weights were adjusted to reduce the sum of the squared errors (Chokphoemphun and Chokphoemphun, 2018; Alkronz *et al*., 2019). This procedure gave as result a prediction model of the simulation of sugar-rich foods (PMSSRF).

The adjustment of the ANN parameters included the number of layers and hiding neurons, the type of function of transference, the learning speed, the momentum, and number of patterns. The log-sigmoid transference function and tangential were used to train and activate the neurons.

2.5 Statistical Analysis

A variance analysis ($P< 0.05$) from the experimental results of the variables of study from the SSRF was made to establish the differences between treatments and interactions between variables that affect the process spray drying of the SRF. Likewise, there were performed linear regressions to compare the results between the output variables from the PMSSRF and the experimental of the SSRF, where the determination coefficient (R^2), the value of Fc ($P< 0.05$) of the interdependent variables and the inflation factor of the variance (IFV) obtained from the variance of the regressions (Cuadras 2004) were implemented for such comparison. On the other hand, the performance of these models was obtained through statistical indexes, such as root mean square deviation (RMSE) and the mean bias error (MBE), by equations 4 and 5 (Douglas *et al*., 2009):

$$RMSE = \sqrt{\left(\frac{1}{n}\right)\sum_{i=1}^{n}(Xe_i - Xp_i)^2} \quad (4)$$

where the RMSE is the square root of the average error; is the number of the tests, Xe_i is the experimental result of the SSRF and Xp_i is the output result of the PMSSRF model.

$$MBE = \left(\frac{1}{n}\right)\sum_{i=1}^{n}(Xe_i - Xp_i) \quad (5)$$

where MBE is the average bias error; The rest of the symbols indicates the same that the equation (4).

The RMSE is a performance indicator of a model in a certain period and the value is always positive; while the MBE gives information of the long-term behavior of the correlations, which allows a comparison of the real deviation between forecasted and measured values, end to end (Gunhan *et al*., 2005) in both cases, the cero is ideal (Segura-Castruita and Ortiz Solorio, 2017).

On the other hand, an orthogonal regression was performed with the objective of establishing if the results that the PMSSRF were equivalents or predicted the results that were obtained experimentally from the SSRF. In this case, the values of the model PMSSRF were considered as the independent variable and the experimental results from the SSRF study as an independent variable. The parameters of the regression were helpful to determine what was mentioned above since the conditions to follow are the following: The confidence interval (CI) of the slope must contain the number 1 and the CI from the intersection must contain the 0, considering the CI at a 95% in both cases and assuming that the dependent and independent variables have the same variance (Segura-Castruita and Ortiz-Solorio, 2017). The data processing was made in the Minitab Software 17 (2017).

3 Results and discussion

3.1 Performance

An analysis was carried out to determine the influence of the study variables about the variable R to find which the main influencing variables and their optimal conditions are to obtain a higher yield from the SSRF process spray drying.

The best treatment was the one with the highest yield and it was the experiment with T-180 ° C with

15% -Mdx 0% -F, 0% -G, 100% -S, 1% -OA with which a 93.44% R. The input variables that influence R, are Mdx (P> 0.000), F, (P> 0.001) and S (P> 0.0014), the Mdx variable shows an increase in R, proportional to the amount of Mdx added. However, it mentions that you must add a certain amount of Mdx to prevent excessive amounts of Mdx from adhering to the product (Villalobos-Castillejos *et al*., 2018; Yinbin *et al*., 2018; Kaderides and Goula, 2019; Kang *et al*., 2019), all treatments above 10% by weight * volume-1 (wv-1) of Mdx do not present drying problems in any SSRF; With respect to F, when we have a higher concentration in the SSRF, it presents problems of adhesion to the drying walls, which causes a low or no yield, this agrees with that established by Bhandari *et al*. (1993), this is related to the low Tg and when there is a concentration greater than 50% wv-1 F, it is not possible to obtain powder unless you add more than 15% wv-1 of Mdx, being the only variable that can be modified (Samborska, 2019), however, when the S is presented in a higher concentration in the SSRF, a better yield is obtained and it is the simplest sugar to dry of the 3 that are addressed in this study because its Tg is greater than those of the rest. When SRF have low or no S concentrations, it may show low or no yield (Singh *et al*., 2019), the amount of Mdx required for a successful R depends on the composition of the SRF (Robaina *et al*., 2019).

3.2 Physic and chemical Properties

Regarding WA, SSRF shows significant differences (P> 0.05) in the input variables T (P> 0.000), F (P> 0.001) and G (P> 0.014), where the WA range is (0.057-0.357), this range is acceptable for powdered food products (Pereira *et al*., 2020); while the SSRF dried at 190 ° C showed less WA since there was a longer residence time within the drying time. However, for H a significant difference was observed in the input variables T (P> 0.001), Mdx (P> 0.23) and G (P> 0.015), of which two of these variables influenced the WA because they were related, since, in the drying, the temperature influences the loss of water, which shows low humidity and water activity, the range obtained was (0.1660 to 0.2119) (Bandhari *et al*., 1997; Chavez-Rodriguez *et al*., 2016; Limpiäinen *et al*., 2018; Villegas-Santiago *et al*., 2020).

The Tg analysis (P> 0.05) showed significant differences in the F variables (P> 0.000), S (P> 0.000) and Mdx (P> 0.000). Likewise, when F increased its concentration, the Tg from the SSRF diminish. On the other hand, the S has an inverse behavior, being this more favorable to avoid stickiness issues in the spray drying process. However, the Mdx when the greater is its concentration, the Tg increased to all SSRF (Bonilla-Ahumada *et al*., 2018).

3.3 ANN prediction spray drying of SRF

The PMSSRF conditions that selected were 4 layers of 10-16-14-10 respectively. As seen in figure (1). The log-sigmoid and tangential transfer functions were the best transfer functions based on the results of training errors and cross-validation. These algorithms provide a numerical solution to the problem of minimizing a function nonlinear (Hermannseder *et al*., 2017). Artificial neuron transfer functions make it difficult for results to reach a very large magnitude that can disable ANN and inhibit training which has a significant influence on ANN learning and performance (Przybył *et al*., 2018). Regarding neurons in the layers, few hidden neurons reduce the ability of ANN to map the input/output relationship.

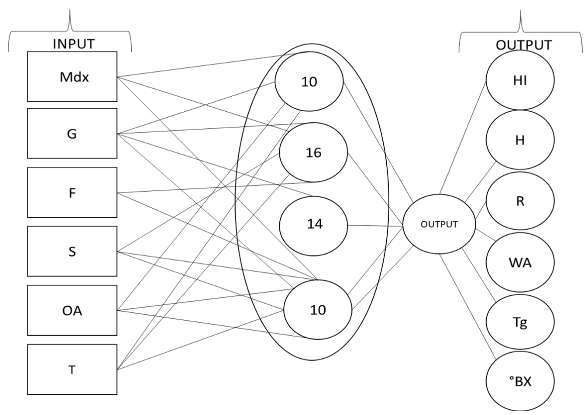

Fig. 1. ANN PMSSRF diagram.

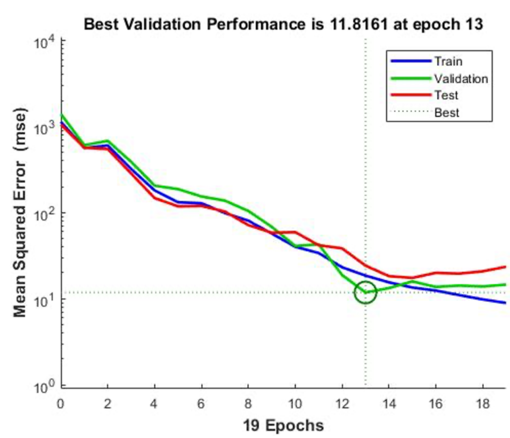

Fig. 2. ANN PMSSRF model validation.

However, ANN with too many hidden neurons are over-trained and the networks learn insignificant details, therefore, they produce an overfit (Pradhan *et al*., 2020), behavior similar to the behavior of the times and I can increase or decrease the error (Castro *et al*., 2018).

Figure 2 shows the validation against the number of training periods for the selected network. This figure shows that the error in training and cross-validation had a descending form, the errors were fed back to the neurons and were used to adjust the weights so that the error is reduced by iteration and the neural model gets closer and closer to produce the desired output. Furthermore, it is clear from this figure that the ANN model was successfully trained, indicating that the selected ANN topology was able to adequately establish the relationship between input and output parameters (Janjai *et al*., 2018; Brusamarello *et al*., 2020).

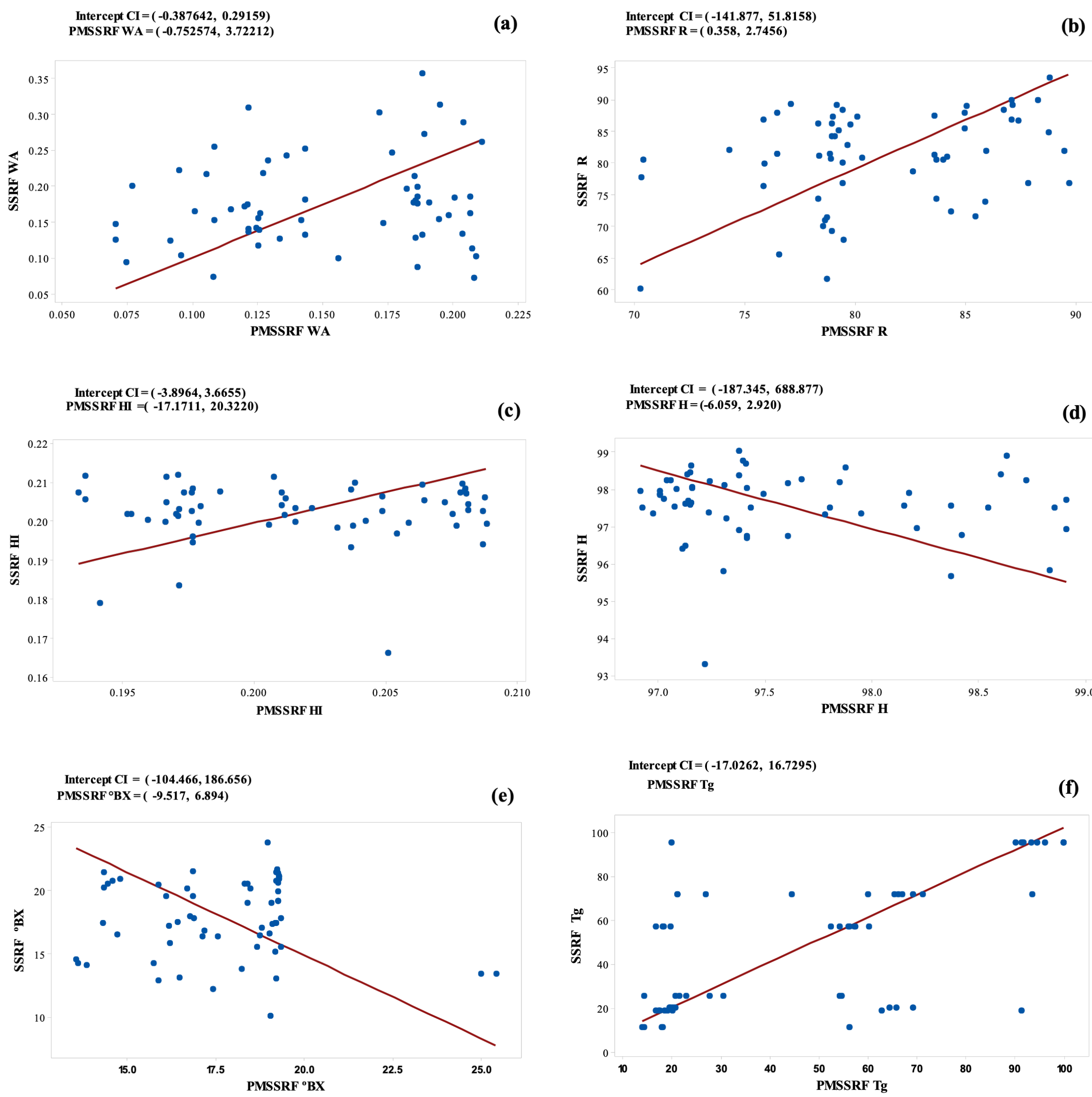

Fig. 3. Orthogonal regressions: a) relation between PMSSRF WA and the validation data (REAL) WA; b) relation between PMSSRF R and REAL R; c) relation between PMSSRF HI and REAL HI; d) relation between PMSSRF H and REAL H; e) relation between PSSRF °BX and REAL °BX; relation between PSSRF Tg and REAL Tg.

Table 1. Predictive capacity of the PMSSRF.

PARAMETER	R	H	WA	HI	Tg	ºBX	Mdx
MBE	0.0027	0.01	-0.025	-0.00065	1.1	-0.096	-0.008
RMSE	0.073	1.14	0.073	0.0089	25.25	3.85	0.154
R^2	0.319	-0.09	0.169	0.022	0.619	-0.041	0.1

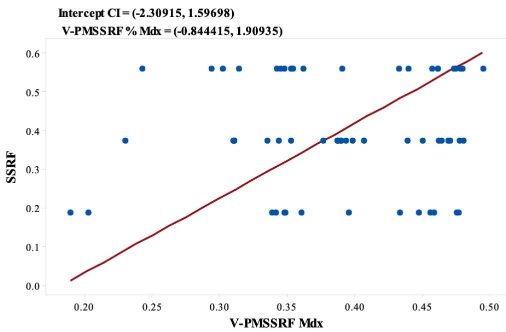

Fig. 4. Orthogonal regression regarding PMSSRF %Mdx and REAL %Mdx.

The PMSSRF model was compared to SSRF in order to measure its predictive capacity; every output variable complies with the CI condition (95%), both for the slop as for the intercept (figure 3 (a), (b), (c), (d), (e), (f)); thus, there isn't evidence that indicates that predicted values from PMSSRF are similar to SSRF; in such way that is deducted that there is no evidence that the model calculates different data than real.

On the other hand, the result of the inverted model PMSSRF were reversed two variables, Mdx changed input variable to output variable and R changed from output variable to input variable, this to establish the model PMSSRF reversed (V-PMSSRF), in order for the model to calculate the percentage Mdx need to obtain the expected performance. In such a way the results of the reversed model once compared to SSRF comply with the condition factors figure (4); thus, it may be simulated the amount of Mdx to be used establishing the sugar concentration from the SSRF and the referential expected performance.

The MBE, in general, shows an ideal condition (closer to 0), being the best for the output variable HI (-0.00065), while the R had the greater error (Table 1). The RMSE shows that this model calculates with low error variables H, WA, HI, °BX, R, Mdx, while the variable Tg has a greater error (25.25). Thus, the R^2 was low due to the behavior of the model is not linear.

The result of R^2 indicates the low linear relation of the drying process from SRF. However, when the orthogonal regression test was made the error was considered in the dependent variables (data from the proposed model) and independent (REAL), when generally in the regression analysis it is considered only the error in the independent variable so that this procedure is recommendable (Lim and Keles, 2018) where there could exist error in the measurement of the dependent and independent variables. This is evidence of the applicability of ANN models to simulate complex and non-linear dynamic systems such as the drying process. This indicates that the developed PMSSRF model can accurately track experimental data and can certainly replace mathematically constitutive models for prediction of exercise from the spray drying process, as it is trained with experimental data and automatically improved through learning. Furthermore, ANN models can improve their performance by relearning new data with or without new processing conditions (Janjai *et al.*, 2018). A properly trained PMSSRF ANN model uses only one set of weights for all drying conditions and is capable of simultaneously producing all outputs. Unlike the empirical models that are applicable to the prediction of data in the simulated range, a trained ANN can estimate the behavior of the process both inside and outside the simulated range. Of course, the empirical models are physically explainable, while the structure of the PMSSRF is difficult to interpret (Kaveh *et al.*, 2018).

Conclusions

In general, the percentage of Mdx needed for a successful dry depends on the composition of the product, drying temperature and expected performance, and it is based mostly in the test experience of trial and error and on the operator; nevertheless with the proposed model it is intended not to need the operators experience, but only knowing the product's composition and expected performance we may calculate the amount of Mdx needed to dry and obtain the whished physio-chemical properties. The proposed model in the current study showed that the input variables T, Mdx, F, G, S and OA may be utilized in ANN models to calculate the spray drying process. Likewise, the Mdx influences the drying process, in such way that when its concentration increases the drying process becomes easy and it is the only variable that may be modified in the process since fruit juice has specific concentrations depending on the fruit or its combination. On the other hand, the orthogonal regression ended up being a statistical tool useful in the model comparison through SSRF, such as PMSSRF. Likewise, based on RMSE, MBE and the orthogonal regression, the model to calculate the spray drying process of SSRF is appropriate. The results of this method are similar to the ones obtained with Bhandari *et al*. (1997), Youssefi *et al*. (2009) and Chaurasia *et al*. (2019), with the advantage of, this model predicts all combinations that may form the SRF in combination with Mdx and not only one specific. So, the V-PMSSRF model that calculates values of Mdx or R, H, AA, HI, Tg and °BX for each SRF that is submitted to the spray drying.

Nomenclature

F	Fructose
G	Glucose
S	Sucrose
OA	Organic Acid
Mdx	Maltodextrin
SRF	Sugar-Rich Foods
SSRF	Simulation of Sugar-Rich Foods
T	Temperature
Tg	Glass Transition Temperature
°BX	Brix degrees
HI	Hygroscopicity index
WA	Water Activity
R	Yield
ANN	Artificial Neural Networks
PMSSRF	Prediction Model of Simulation of Sugar-Rich Foods
V-PMSSRF	Reversed Prediction Model of Simulation of Sugar-Rich Foods

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