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Artificial Neural Network (ANN) and mathematical modeling of hydration of corn cereal with milk

Rede Neural Artificial e Modelagem matemática na hidratação de cereais matinais com leite

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The crunchiness of breakfast cereal is associated with the freshness and quality of the product, and its loss can cause rejection to consumption. So, it is important to know the hydration kinetics of different food products, as well as the influence of process conditions (such as temperature and time) on their rates. The objective of this work was to evaluate the effect of hydration on the physical-chemical properties of the milk-hydrated cereal by studying the hydration kinetics with the application of empirical models and Artificial Neural Networks (ANN). Hydration was conducted in 3 cereal/milk proportions, 3 immersion temperatures. The Peleg models was used, and the physical-chemical responses and kinetic parameters of the hydration process were considered for modeling and simulation using RNA. For the hydrated cereal, analyzes of moisture, ashes, lipids, and crude fiber were carried out. For the milk the analyzes were soluble solids and lipids. The treatments used in hydration had a significant effect ($p < 0.05$) on all physical-chemical properties of breakfast cereal. Of the two models, the Peleg model best described the kinetics of milk absorption in the cereal. However, the use of Artificial Neural Network was more efficient in adjusting the data for absorption.
Keywords: quality, technology, hydratation process.

A crocância do cereal matinal está associada ao frescor e à qualidade do produto, e sua perda pode ocasionar rejeição ao consumo. Portanto, é importante conhecer a cinética de hidratação de diferentes produtos alimentícios, bem como a influência das condições do processo (como temperatura e tempo) em suas taxas. O objetivo deste trabalho foi avaliar o efeito da hidratação nas propriedades físico-químicas do cereal leite hidratado por meio do estudo da cinética de hidratação com a aplicação de modelos empíricos e Redes Neurais Artificiais (RNA). A hidratação foi conduzida em 3 proporções cereal/leite, 3 temperaturas de imersão. Os modelos Peleg foram usados, e as respostas físico-químicas e os parâmetros cinéticos do processo de hidratação foram considerados para modelagem e simulação usando RNA. Para o cereal hidratado, foram realizadas análises de umidade, cinzas, lipídios e fibra bruta. Para o leite, as análises foram sólidos solúveis e lipídios. Os tratamentos utilizados na hidratação tiveram efeito significativo ($p < 0{,}05$) em todas as propriedades físico-químicas do cereal matinal. Dos dois modelos, o modelo Peleg melhor descreveu a cinética de absorção do leite no cereal. Porém, o uso da Rede Neural Artificial foi mais eficiente no ajuste dos dados para absorção.
Palavras-chaves: qualidade, tecnologia, processo de hidratação.

1. INTRODUCTION

Breakfast cereals are products obtained by extrusion technology, and the grains most commonly used for their production in the food industry are rice, wheat, corn and oats. The crunchiness of breakfast cereal is associated with the freshness and quality of the product, and its loss is one of the causes of rejection of consumption [1, 2]. However, such products readily absorb moisture, and may undergo undesirable changes when exposed to the atmospheric environment, or hydrated with milk or other liquids. The mechanism of moisture absorption is related to the movement of water inside the cereal, and its ability to hydrate. The water affects the texture of dry and crunchy foods by plastification and softening of the starch/protein matrix, which alters the mechanical resistance of the products [3].

The hydration process is an important unitary operation in dry foods because it describes their properties during cooking, extraction, fermentation, germination and/or feeding. Therefore, it is important to understand the hydration kinetics of different food products, as well as the influence of the process conditions (such as temperature and hydration time) on their rate [4].

In this context, mathematical models are important for designing, simulating and optimizing the conditions of hydration processes [5]. The Artificial Neural Network (ANN) is a computational and nonlinear statistical technique capable of solving a range of highly complex problems and heltp to controll of food processing operations through a Multilayer Perceptron neural network (MLP). An MLP type consists of an input set, which forms the input layer, one or more hidden layers and an output layer [6, 7, 8].

In this way, the objective of this work was to evaluate the effect of hydration on the physical-chemical properties of breakfast cereal hydrated with milk and to study the kinetics of breakfast cereal hydration by the application of empirical models and Artificial Neural Networks (ANN).

2. MATERIAL AND METHODS

A For the present work, corn cereal was used, with no added sugar and UHT whole milk, both obtained from local shops in the city of Palmas, Tocantins, Brazil.

2.1 Hydration of breakfast cereal

Hydration was conducted under the following conditions: three cereal/milk proportions (1/5, 1/10 and 1/15) and three immersion temperatures (35 °C, 45 °C and 55 °C). The procedure was done in water bath (TECNAL, model TE-0541-1), with temperature control. The hydration was done in triplicate (with 2 replicates), and occurred during 2 hours, with removal of the cereal at different immersion times (15, 30, 45, 60, 75, 90, 105 and 120 minutes) for analysis of the kinetics of absorption of milk. The cereal was removed from the immersion and placed on filter paper to eliminate excess milk, and then weighed. It then returned to immersion for continuity of the process.

2.2 Physical-chemical characterization

The analysis carried out in the cereal were: moisture, ash, lipids and crude fiber. For the milk, the analyzes were: soluble solids and lipids. Following the methodology of the Adolfo Lutz Institute (IAL, 2008).

2.3 Statistical analysis

For data treatment, the analysis of variance was used, followed by the Scott-Knott test to test the hypotheses of the treatments and their interactions. Statistical analyzes were conducted using the SISVAR software [9].

2.4 Kinetic Modeling

The milk content at a given time after the start of the experiment was calculated based on the increase in mass of the samples in relation to the initial mass. In order to describe the milk absorption kinetics of the samples: Peleg Model was used.

The Peleg model is represented by Equation 1, where C_1 and C_2 represent the constants of the model [10]:

$$\mathrm{Ut} = \mathrm{U}_0 + \frac{\mathrm{t}}{(\mathrm{C}_1 + \mathrm{C}_2\mathrm{t})} \quad (1)$$

Ut is the moisture content at time t (decimal b.s.); U_0 is the initial moisture content (decimal b.s.); t is the hydration time (min); C_1 is the Peleg constant rate (min/decimal b.s.); C_2 is Peleg's constant capacity (decimal b.s.$^{-1}$).

For modeling and simulation using the artificial neural network, the physical-chemical responses and the kinetic parameters resulting from the hydration process were considered.

For the construction of the neural network, a treatment in the data was necessary. Both input and output data were normalized before powering the network, according to Equation 2:

$$x_{i,normal} = \frac{x_i - \text{minímo}(x_i)}{\text{máximo}(x_i) - \text{minímo}(x_i)} \quad (2)$$

The network performance was measured by the linear correlation coefficient (R^2), the mean relative error (P) and the standard error of the estimate (SE).

The physicochemical analyzes of the cereal and milk followed the generic scheme presented in Figure 1, where the independent variables (proportion, temperature and time) were used as input, and the dependent variables (lipids, moisture, ashes, soluble solids and fibers) were individually adopted as output (X).

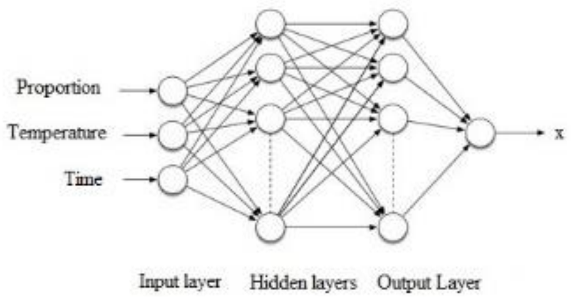

Figure 1. Generic ANN construction scheme for physical-chemical characterization.

3. RESULTS AND DISCUSSIONS

3.1 Physical-chemical characterization

Tables 1 and 2 shows the results of the analysis of variance (ANOVA) for the physical-chemical analyzes performed in the breakfast cereal and in the milk used as the absorption fluid in the hydration process. The values were significant ($p < 0.05$) in all sources of variation and analyzes, indicating that there were differences in the results obtained from the hydration of the cereal. For all analyzes, the coefficient of variation (CV) was low, indicating accuracy of the obtained data.

Table 1. ANOVA of the physical-chemical characterization of breakfast cereal.

		Medium Square of Variables			
Sources of Variation	**DF**	**Moisture**	**Lipids**	**Ash**	**Crude Fiber**
Proportion (F1)	2	286.403417*	13.032651*	5.605489*	0.065425*
Temperature (F2)	2	61.809950*	7.540935*	7.035862*	0.125595*
Time (F3)	7	50.205464*	0.227500*	0.421097*	0.039712*
F1*F2	4	14.106177*	2.761124*	0.070805*	0.090226*
F1*F3	14	4.026195*	0.064837*	0.125375*	0.043836*
F2*F3	14	3.897173*	0.564406*	1.397838*	0.080564*
F1*F2*F3	28	2.500677*	0.155931*	0.161589*	0.086278*
Error	144	0.014947*	0.005996*	0.007445*	0.005909*
Total	215				
CV (%)		0.17	3.04	3.64	5.57
Overall mean		71.8406019	2.5456944	2.3724537	1.3811157

**Significant at the 5% probability level (p <0.05), by the F test.*

Table 2. ANOVA of the physical-chemical characterization of milk.

Sources of Variation	Medium Square of Variables		
	DF	Soluble Solids	Lipids
Proportion (F1)	2	185.083380*	4.931878*
Temperature (F2)	2	119.694525*	1.735906*
Time (F3)	7	53.998042*	0.290811*
F1*F2	4	3.977546*	0.327507*
F1*F3	14	3.596197*	0.112499*
F2*F3	14	1.208176*	0.066343*
F1*F2*F3	28	0.694947*	0.095606*
Error	144	0.003449*	0.007512*
Total	215		
CV (%)		0.36	2.75
Overall mean		16.2629630	3.1524074

**Significant at the 5% probability level (p <0.05), by the F test.*

Tables 3, 4 and 5 show the results for the physico-chemical analyzes of the cereal and milk used during hydration at the different temperatures and proportions analyzed.

The increase in temperature caused an increase in moisture content, regardless of cereal/milk proportion analyzed, indicating that this factor affects the kinetics of milk absorption in the cereal (Table 3). The temperature influences the diffusion of liquids inside the food, resulting in increased volume. At higher temperatures, the increase in volume is higher, resulting in greater space for water absorption [11, 12, 13]. Similar behavior was found when analyzing the kinetics of soy hydration for a period of 450 minutes at three different temperatures and concluded that temperature and time had a significant effect, increasing the moisture content of the grain [14]. This was also observed during the hydration of chickpeas [12].

Table 3 shows the result of the Scott-Knott test when the lipid content of the breakfast cereal was analyzed. Evaluating the effect of temperature, cereal contents were higher at higher temperatures. Analysis the hydration of pea grains, concluded the increase of mass transfer with the elevation of temperature [15]. In general, it is observed that the increase in the proportion and consequently the amount of milk in the absorption system caused an increase in the lipid content at all temperatures. When the milk was analyzed, contrary behavior was observed, with a decrease in the lipid content of this fluid when the amount of milk in the process was higher (Table 5), indicating a possible mass transfer between the cereal and the milk during hydration. Observed that the contents found for the hydrated breakfast cereal (Table 3) are much higher than that of breakfast cereal without milk, which is around 0.8% [16]. Because it is a food with a lipid content around 3.35% [17], milk may have contributed to the increase of lipids in the cereal. When analyzed the effect of time, it was observed oscillations in the lipid content of the cereal, indicating the search for equilibrium by the system. Evaluating the temperature effect, the increase of the temperature caused an increase in the lipid content, indicating that the mass transfer is greater with the increase in temperature. Such behavior is explained by [18] who evaluated the hydration kinetics of breakfast cereals with skimmed milk and without lactose and observed that the mass transfer is greater at higher temperatures, but tends to decrease with increasing water concentration in the cereals, because the system tends to balance itself.

Table 3. Moisture and Lipids of the cereal at the different temperatures and proportion analyzed.

Temperature (°C)	Moisture Mean (%)			Lipid Mean (%)		
	Proportion of Cereal/Milk					
	1:5	1:10	1:15	1:5	1:10	1:15
35	69.06 ^{a}	70.66 ^{a}	73.54 ^{a}	1.95 ^{aB}	2.24 ^{bA}	2.81 ^{cA}
45	69.51 ^{b}	71.46 ^{b}	73.68 ^{b}	1.54 ^{aA}	2.59 ^{bB}	3.04 ^{Cc}
55	70.68 ^{c}	73.99 ^{c}	73.95 ^{c}	2.82 ^{aC}	2.87 ^{bC}	3.01 ^{cB}

Moisture: Scott-Knott's test at the 5% probability level. Averages followed by the same letter in the column do not differ statistically from each other. Lipids: Scott-Knott's test at the 5% probability level. Averages followed by the same letter in the column do not differ statistically from each other.

Table 4 shows the result of the Scott-Knott test when analyzed the ash content of the cereal. The ash content decreased as the proportion increased. It is observed that the fiber content decreases with increasing milk quantity in the system, as well as decreases with increasing temperature. However, the milk has no fiber content for a possible mass transfer, and the crude fiber is stable at temperature, so that the methodology for its determination has the final step of burning in a muffle at 550 ºC. Therefore, this minimum variation that occurred between the factors can be explained by the variability in relation to the contents of the samples themselves during the experiment. Regarding the effect of time, the fiber content remained stable during hydration, and there were no significant increases or reductions, due to the fact that the milk does not have fibers in its composition. Therefore, there was no addition of this constituent in the system (Table 4).

Table 4. Ashs and Crude Fiber content of the cereal at the different temperatures analyzed.

Temperature (ºC)	Ashs Mean (%)			Crude Fiber Mean (%)		
	Proportion of Cereal/Milk					
	1:5	1:10	1:15	1:5	1:10	1:15
35	2.26 ^{cA}	1.95 ^{bA}	1.83 ^{aA}	1.46 ^{cC}	1.37 ^{bB}	1.36 ^{aC}
45	2.83 ^{cB}	2.42 ^{bB}	2.23 ^{aB}	1.37 ^{bB}	1.39 ^{cC}	1.34 ^{aB}
55	2.93 ^{cC}	2.55 ^{bC}	2.31 ^{aC}	1.35 ^{cA}	1.32 ^{bA}	1.31 ^{aA}

Scott-Knott's test at the 5% probability level. Averages followed by the same letter do not differ statistically from each other. Lines: lowercase letters. Columns: uppercase letters.

Table 5 shows the result of the Scott-Knott test when analyzed the soluble solids content of the milk during the heat and mass transfer process. Regarding the effect of the proportion, it is observed at all temperatures that the solids content decreases as the proportion increases, as the mass transfer is greater at higher temperatures, but decreases with the increase of the water concentration in the grain [19]. An increase of soluble solids was observed during the absorption process in all the temperatures studied indicating the mass transfer due to contact between milk and cereal.

Table 5. Lipid content of the milk at the different temperatures analyzed.

Temperature (ºC)	Lipid Mean (%)			Soluble Solids Mean (ºBrix)		
	Proportion of Cereal/Milk					
	1:5	**1:10**	**1:15**	**1:5**	**1:10**	**1:15**
35	3.20 ^{cA}	3.02 ^{bA}	2.89 ^{aB}	16.03 ^{cA}	14.48 ^{bA}	13.81 ^{aA}
45	3.65 ^{cC}	3.35 ^{bC}	2.94 ^{aC}	18.94 ^{cB}	16.60 ^{bB}	15.23 ^{aB}
55	3.33 ^{cB}	3.11 ^{bB}	2.83 ^{aA}	19.04 ^{cC}	16.68 ^{bC}	15.53 ^{aC}

Scott-Knott's test at the 5% probability level. Averages followed by the same letter do not differ statistically from each other. Lines: lowercase letters. Columns: uppercase letters.

4. KINETIC MODELING

During the process, higher absorption was observed in the first fifteen minutes of hydration, followed by slower absorption, system balance and decreased milk content. Similar behavior was observed in Alpiste grains at the beginning of the hydration process, where hydration has a high-water absorption rate that tends to decrease with time, as the grain approaches equilibrium [11]. Table 6 shows the constants obtained from this model, as well as the predicted values of the equilibrium moisture (Ueq) and the values of the coefficients of determination (R^2), relative mean error (SE) and standard error of the estimate (P) for Peleg model, adjusted during the hydration of the cereal.

Table 6. Parameters of the Peleg model applied to the moisture absorption kinetics and statistical indices for the modeling of breakfast cereal hydration.

Peleg Model							
Proportion	**T (ºC)**	**C_1**	**C_2**	**U_{eq}**	**R^2**	**SE**	**P (%)**
	35	0.22	0.0274	46.56	1.00	0.48	0.75
1:5	45	0.19	0.0272	46.80	1.00	0.99	0.84
	55	0.12	0.0270	47.16	0.99	1.10	1.78
	35	0.17	0.0299	43.49	1.00	0.56	1.51
1:10	45	0.08	0.0301	43.26	0.99	1.36	1.92
	55	0.01	0.0312	42.15	0.99	0.96	2.27
	35	0.16	0.0303	43.08	0.99	1.25	2.21
1:15	45	0.06	0.0296	43.89	1.00	1.81	1.27
	55	0.01	0.0295	43.94	0.99	1.59	2.15

The constant C1 of Peleg model is related to the mass transfer rate, and the lower their values, the higher the initial rates of water absorption [20]. According to Table 1, the values of C1 decreased with increasing temperature, indicating that the absorption is higher at higher temperatures. It is observed that the values also decreased as the proportion increased, showing that when a larger amount of milk was added to the system, the absorption was higher at the beginning of the process. Some authors have proposed that the mechanism of transport of fluids in solid foods occurs by liquid diffusion, especially in fine-structure solids with small holes filled with air, which is the case of breakfast cereal [21].

The C2 constant of the Peleg model is related to the maximum water absorption capacity, and the lower its value, the greater the water absorption of the product [20]. In the hydration of the breakfast cereal, this constant varied little, but followed the same behavior of C1 indicating that the cereal has greater capacity of absorption when submitted to higher temperatures. When the effect of the ratio was analyzed, the behavior was contrary to that of C1, and the maximum absorption capacity was obtained to a lesser extent. The Ueq corroborates with parameter C2, showing higher when the cereal has greater capacity of milk absorption. Analysis of the hydration of Alpiste grains concluded that the increase in temperature causes the absorption capacity to be greater, as well as the equilibrium humidity [11]. There was also an increasing trend in parameter C2, when analyzing the hydration of quinoa and lentil seeds, respectively [22, 23].

The values of the coefficients of determination (R^2), relative mean error (SE) and standard error of the estimate (P) for Peleg model, adjusted during the hydration of the cereal, are presented in Table 6.

When the values of the correlation coefficient (R2) presented values equal or superior to 0.982 and standard deviations lower than 1,423, they elevate the confidence level of the adjustments [24]. Thus, Peleg's model had a good fit to the experimental data, and better represented the data when the temperature was lower (obtaining higher value of R^2, and lower values of SE and P) [20] observed a better fit of the Peleg model for lower temperatures and attributed the fact to the greater loss of solids that occurs in this type of process at higher temperatures, which is not accounted by the model.

Figure 2 shows the absorption of milk in the breakfast cereal through adjustment by ANN. As previously mentioned, when the values of the correlation coefficient (R2) presented values equal or superior to 0.982 and standard deviations lower than 1,423, they elevate the confidence level of the adjustments [24]. Comparing the mathematical Peleg model with the adjustment by Artificial Neural Networks, we can see that the latter obtained better values of the SE and P parameters, and despite presenting a lower R^2 than Peleg (Table 9), was still a satisfactory value (0.98). That is, the adjustment for Neural Networks too obtained a satisfactory result.

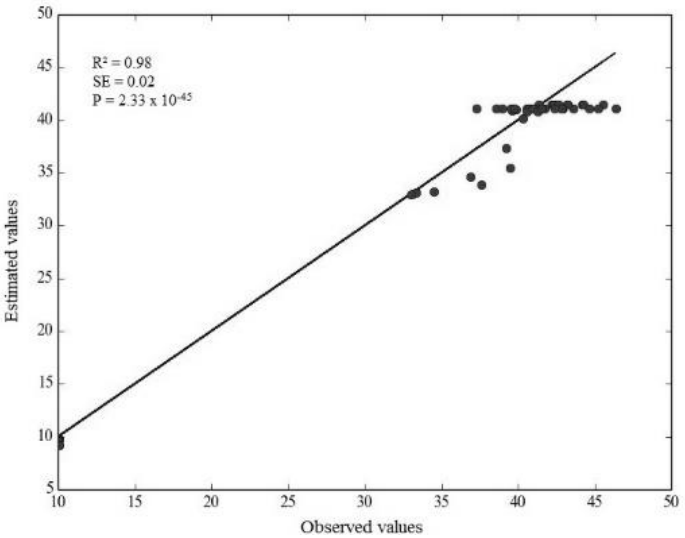

Figure 2. Correspondence between experimental and estimated ANN values for milk absorption in the breakfast cereal.

Figures 3 shows the correlation graphs between the experimental (observed) and estimated values by the Artificial Neural Network for the physical-chemical analyzes of the breakfast cereal.

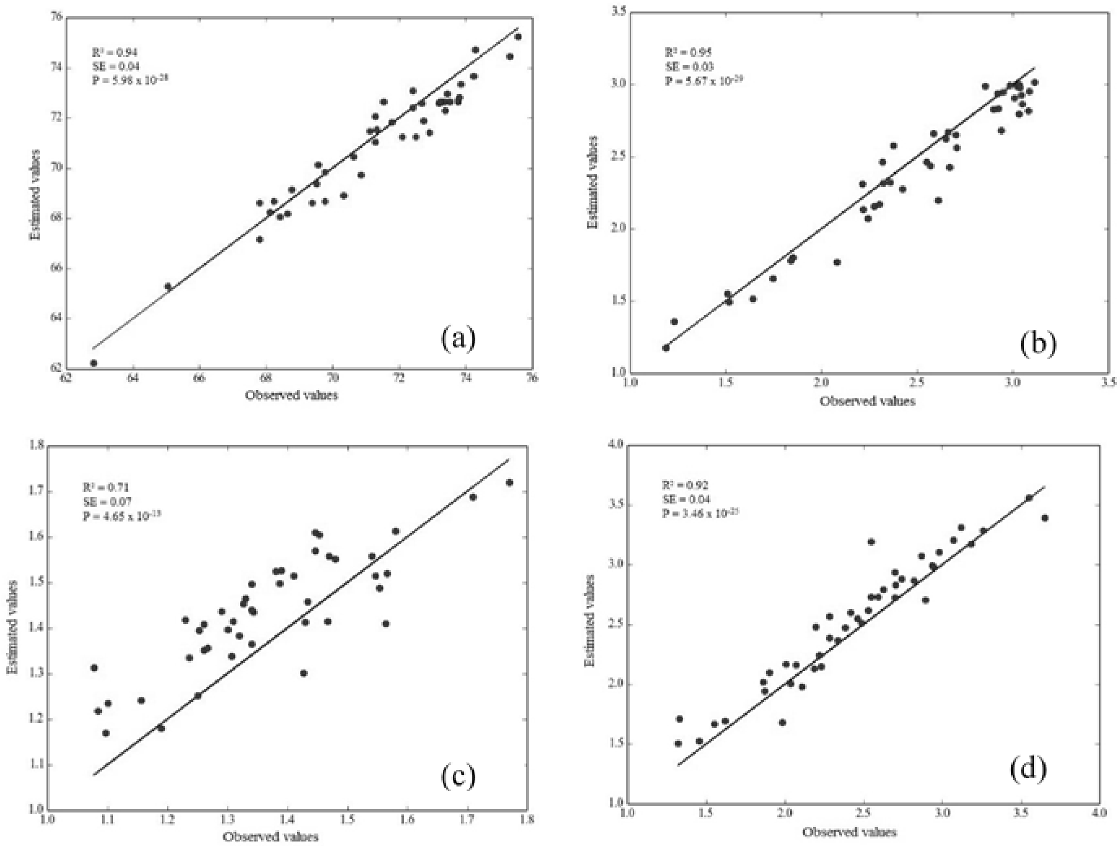

Figure 3. Correspondence between the experimental and estimated ANN values. (a) breakfast cereal moisture, (b) breakfast cereal lipids, (c) breakfast cereal crude fiber and (d) breakfast cereal ash.

It was observed that the modeling by Artificial Neural Network was efficient in adjusting the obtained data, having good correlation coefficients (with the exception of crude fiber analysis), and low values of relative mean error (P) and standard error of the estimate (SE). This tool has been used by many authors because of their effectiveness in data fitting [8, 25, 26].

Figures 4 show the correlation graphs between the experimental (observed) and estimated values by the Artificial Neural Network for the physical-chemical analyzes of the hydration milk.

It can be noticed that the modeling by Artificial Neural Network was also efficient in adjusting the data obtained for the milk analysis, having good correlation coefficients, and low values of mean relative error (P) and standard error of the estimate (SE). This methodology proves to be quite effective for solving problems in food processing [7].

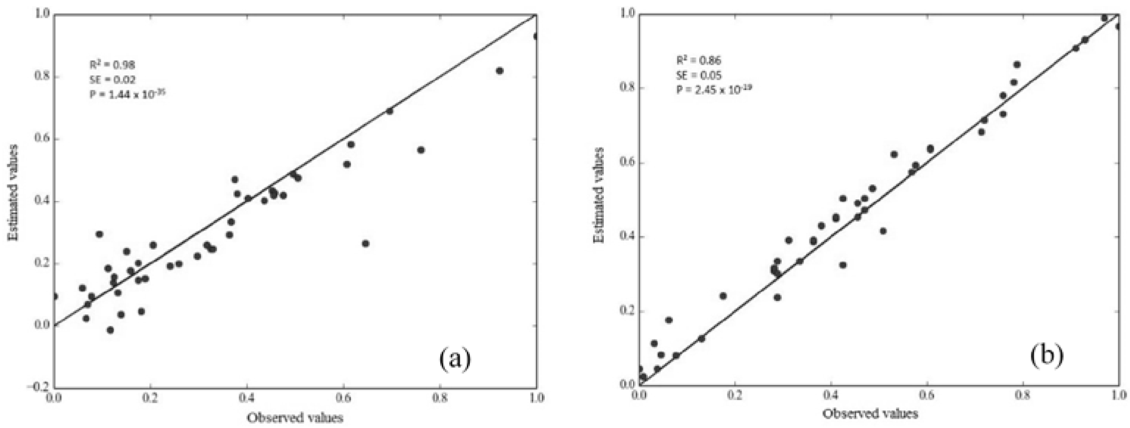

Figure 4. Correspondence between the experimental and estimated ANN values. (a) soluble solids of the hydration milk, (b) lipids of the hydration milk.

With the technological advance, there is the search for computational procedures that aim at the best performance and that, as far as possible, present relatively low cost. ANN's are mathematical models based on the functioning of the biological nervous system, and have been used in several areas to replace the regression models, often presenting superiority in the accuracy of the estimates of the variables of interest. This tool is very advantageous, because it is an alternative for complex functions, does not require detailed information about the system to be modeled, tolerates data loss and allows the adjustment of phenomena of a linear and non-linear nature. Another advantage of ANN is that while the Peleg and others mathematical models use as input only data related to moisture and absorption, and run the model separately for each treatment, the neural network allows to correlate all treatments at once in the input of the model, and can obtain as a response not just parameters of absorption, but also physical-chemical parameters (which are not possible in other models), since in food processing it is important consider the nutritional loss that occurs during the process [7, 8].

5. CONCLUSION

The treatments used in hydration (proportion, temperature and time) caused a significant effect ($p < 0.05$) on all physical-chemical properties of breakfast cereal hydrated with milk. The Peleg model best described the kinetics of milk absorption in the cereal at the temperatures and proportions investigated, and obtained good adjustments to the experimental data. However, the application of the Artificial Neural Network to the physical-chemical characteristics of the cereal and milk represented more satisfactorily the absorption kinetics.

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