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ORIGINAL ARTICLE

Modelling of sorghum soaking using artificial neural networks (MLP)

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Abstract

Introduction Artificial neural network is a technique with flexible mathematical structure which is capable of identifying complex non-linear relationship between input and output data. *Objectives* The aim of this study was evaluation of artificial neural network efficiency for simulating the soaking behaviour of sorghum kernel as a function of temperature and time. *Methods* In this study, soaking characteristics of sorghum kernel was studied at different temperatures (10, 20, 30, 40 and 50 °C) by measuring an increase in the mass of sorghum kernels with respect to time. A multilayer perceptron neural network was used to estimate the moisture ratio of sorghum kernel during soaking at different temperatures and a comparison was also made with the results obtained from Page's model. The soaking temperature and time were used as input parameters and the moisture ratio was used as output parameter. *Results* Results showed that the estimated moisture ratio by multilayer perceptron neural network is more accurate than Page's model. It was also found that moisture ratio decreased with increasing of soaking time and increased with increasing of soaking temperature. *Conclusion* The artificial neural network model was more suitable than other models for soaking behaviour estimation in sorghum kernel.

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Introduction

Sorghum [*Sorghum bilcolour* (L.) Moench] is the fifth leading cereal crop in the world, with an estimated production of some 65 million metric tons in the year 2008 (Daraei Garmakhany *et al*., 2011). It is adapted to the semi-arid and subtropical agro-economic conditions of Africa where 55% of the world's sorghum is grown (Belton & Taylor, 2004) and most of it is used as food and feed. However. recent interests in the substitution of barley malt with sorghum malt in some African countries and the continued development of new sorghum-based products such as baby foods and porridge are likely to result in its increased cultivation (Rohrbach, 2003).

From a processing and engineering point of view, one is interested not only in knowing how fast the adsorption of water can be accomplished, how it will be affected by processing variables (Verma & Prasad, 1999), but also on how one can predict the soaking time under given conditions. Thus, quantitative data on the effect of processing variables are necessary for practical applications to optimize and characterize the soaking conditions, design food processing equipment, and predict water adsorption as a function of time and temperature (Bhattacharya, 1995; Abu-Ghannam & McKenna, 1997). Soaking is a slow process that is controlled by the diffusion of water into the grain (Engels *et al*., 1986).

Artificial neural networks (ANNs) is a mathematical tool, which tries to represent low-level intelligence in natural organisms and it is a flexible structure, capable of making a non-linear mapping between input and output spaces (Rumelhart *et al*., 1986). ANNs have already been applied to simulate processes such as fermentation (Latrille *et al*., 1993), crossflow microfiltration (Dornier *et al*., 1995), and drying behaviour of different food and agricultural materials such as carrot (Erenturk & Erenturk, 2007), tomato (Movagharnejad & Nikzad, 2007), ginseng (Martynenko & Yang, 2006), cassava and mango (Hernandez-Perez *et al*., 2004), green malt (Aghajani *et al*., 2012), but there is no information about the application of ANNs in the simulation of soaking process (in particular for grain). This study was carried out to test and validate the efficiency of ANNs for simulating the soaking behaviour and the effect of temperature and time on the hydration of sorghum kernel. The results were also compared with those obtained from Page's model.

Materials and methods

Sample preparation

The sorghum kernels used in this research were obtained from Seed and Plant Breeding Institute, Karaj, Iran. Samples were cleaned manually to remove foreign materials and broken kernels. The initial moisture content of samples was determined by drying about 5 g of samples in an air convection oven at 103 ± 2 °C until a constant weight was obtained (AOAC, 2006) and was found to be 12.00 (%w.b.). This experiment was repeated three times to determine mean values.

Soaking procedure

Approximately 10 ± 0.5 g of sorghum kernels were placed in 200 mL of distilled water at five different soaking temperatures (10, 20, 30, 40 and 50 °C). Thirty samples along with the soaking water were placed in a water bath (WNB 14, Memmert GmbH Co., East Frisian Island, Germany) with a temperature control accuracy of ± 0.5 °C fixed at the given soaking temperature. The sorghum kernels were soaked at each temperature for 30 h and soaked samples were withdrawn from the water at different time intervals (60 min at the first 6 h and 120 min for 12 h and at the rest of soaking process every 60 min). After reaching each predetermined sampling time, the samples were drained on a paper and the excess water eliminated with adsorbent paper, and the soaked sorghum kernels were weighed with a digital balance (A&D Company, Tokyo, Japan) with 0.001 g accuracy. Moisture content of the samples was calculated based on the increase in sample mass at each predetermined time until the experiment was completed. All experiments were conducted three times to reduce error. The mass uptake was calculated as:

$$WU(\%) = \frac{(W - W_0)}{W_0} \times 100 \quad (1)$$

where WU, W and W_0 are mass uptake, seed mass after and before soaking, respectively.

Analysis of soaking data and soaking models

The effects of soaking time and temperature on water uptake and equilibrium moisture content of sorghum kernels were determined using the analysis of variance method and significant differences of means were compared using the Duncan's test at 95% significant level.

There are different models which might be adequate to describe diffusion behaviour of agricultural materials. Page model (Eq. 2) is one of the most popular models that is used to describe water diffusion into foods and agricultural materials. In the analysis of water adsorption data of sorghum kernel, the moisture ratio (MR) is essential to describe Page model.

$$\mathrm{MR} = \exp\left(-\mathrm{kt}^{\mathrm{N}}\right) \quad (2)$$

$$\mathrm{MR} = \frac{M_t - M_e}{M_0 - M_e} \quad (3)$$

where k and N are the constatnt coefficient, M_t is moisture content (dry basis) at time t, M_e is equilibrium moisture content and M_0 is initial moisture content.

After calculation of the MR, the Page model was fitted to the soaking data. There are several criteria such as coefficient of determination (R^2), mean square error (MSE) and residual plotting to evaluate the fitting of a model to experimental data. The average percent difference between the experimental and predicted values or the mean relative deviation modulus (P) has also been used as a measure of model adequacy (Kashaninejad *et al*. 2009):

$$\mathrm{P} = \frac{100}{n} \sum_{i=1}^{n} \frac{\left|MR_{\mathrm{measured}} - MR_{\mathrm{predicted}}\right|}{MR_{\mathrm{measured}}} \quad (4)$$

Non-linear regression procedure was performed on all soaking runs to estimate the parameters associated with Page model from the experimental data using proc LOGISTIC of SAS Software (2001).

The model constants were then related to the soaking temperatures to obtain functional relationship, which were determined using regression technique. The best model

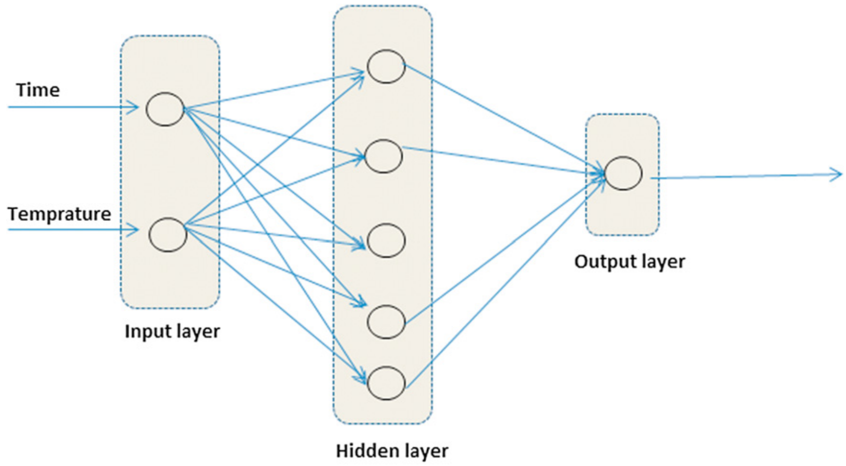

Figure 1 Multilayer perceptron neural network.

describing the soaking characteristics of sorghum kernel was chosen as the one with the highest R^2 and the least MSE and P.

Development of ANNs model

In this paper, multilayer perceptron (MLP) network on back propagation learning rule was used to simulate soaking characteristics of sorghum kernels.

The back propagation network is a multilayer feed-forward neural network with back propagation learning. Here, the network consists of three layers, i.e. the input layer, the hidden layer and the output layer (Figure 1). The input nodes receive the data values and pass them on to the first hidden layer nodes.The input layer consists of two inputs, i.e. temperature and time, and one output layer that consists of one output target, i.e. moisture content.

Each one collects the input from all input nodes after multiplying each input value by a weight, attaches a bias to this sum and passes on the results. However, as the activation function can affect the prediction results, two different sets of comparisons, based on different activation functions, were studied. The first set of comparisons used the results obtained from using a sigmoid tangent function in the hidden layer and a purlin in the output layer. The second set of comparisons used the results obtained from using a sigmoid function in both the hidden and output layers.

Experimental data from this study were used to train and test two ANNs (MLP) for prediction of sorghum kernel MR during the soaking process. Totally, 95 data were collected for the five different soaking temperatures of 10, 20, 30, 40 and 50 °C. For our model, the ratio between the amount of training and testing data was 60:40. For prevention over training of created network in this experiment, the learning rate was varied from [0.1, 0.001]. The studied network was implemented under MATLAB 7.10 software, with the Neural Network Toolbox 4 (The Mathworks, Inc., Natick, MA, USA).

The number of neurons in input and output layers depends on independent and dependent variables, respectively. MR was considered as dependent variable and soaking temperature and time were selected as independent variables. Therefore, one and two neurons were devoted to output and input layers, respectively. The number of neurons in the hidden layer and the parameter a were determined by calibration through several run tests. In this study, one hidden layer including 5–20 neurons was used for the MLP neural networks. The structure of best network was 2:5:1 and

Results and discussion

Effect of soaking time on water adsorption

The moisture content of sorghum kernels calculated at five soaking temperatures during hydration process is shown in Figure 2. A regular increase in water absorption was observed as temperature increased from 10 °C to 50 °C. This phenomenon can be linked to high rate of water diffusion at higher temperature. These observations are in agreement with other studies (Sopade & Obekpa, 1990; Pan & Tangratanavalee, 2003; Kaptso *et al*., 2008; Moreira *et al*., 2008). Figure 2 indicates that the rate of water absorption is initially rapid and then slows down as equilibrium approaches. This asymptotic behaviour is related to the decrease of driving force for water transfer as hydration progresses and the system is close to equilibrium. This effect was also observed during water soaking of rice and lupin (Bello *et al*., 2004; Solomon, 2007).

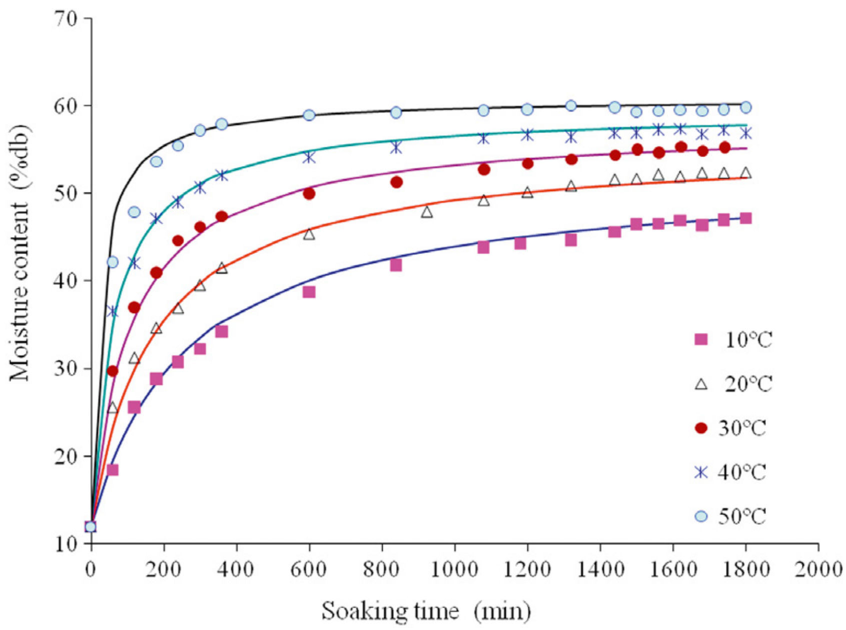

Figure 2 Effects of soaking time and temperature on water uptake of sorghum kernels.

Modelling of water adsorption of sorghum kernel

In this study, soaking characteristics of soghum kernel were studied experimentally. A comparative study was performed between a regression analysis, multilayer feed-forward and radial basis function neural networks to estimate their abilities for prediction of MR. Feed-forward back propagation (FFBP) network was used for mapping between inputs and outputs of patterns. Various threshold functions for all layers were utilized to investigate different threshold functions affecting network optimization. This strategy, together with learning algorithm of Levenberg–Marquardt (LM), was used for FFBP networks. Several topologies were tested, and the best results from each network, training algorithm and threshold functions are represented in Table 1. As can be seen from Table 1, the strategy of FFBP network, LM algorithm with Tangsig-Tangsig threshold functions and five neurons showed the best performance. This is because MSE and R^2 have the better values, experimental and predicted data set and *MSE*.

Table 2 showed the statistical analysis results for Page's model fitted to the soaking data of sorghum kernels. Acceptable R^2 of greater than 0.99 and low MSE and *P*-values were obtained for all experiment runs fitted to the model.

The Page's model coefficients (k and N) for each soaking run were calculated (Table 3). A regular increase in k coefficient was observed as temperature increased from 10 °C to 40 °C. However, an abnormal behaviour was observed at

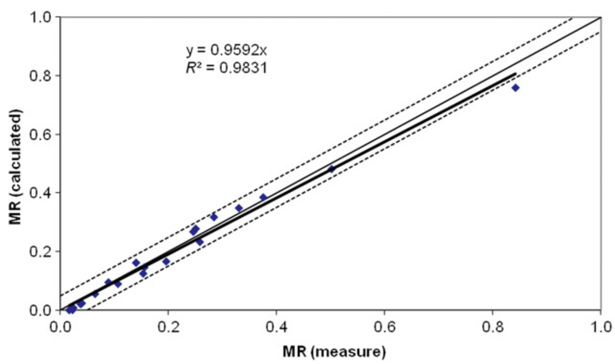

Figure 3 Comparison between measured and calculated values of MR by generalized Page's model. MR, moisture ratio.

50 °C. It may be due to the effect of high temperature inducing softening or adsorption of more water than expected at higher temperatures (Maskan, 2002). Further analysis was performed to describe the temperature dependence of k and N. MR predicted with the generalized Page's model and MLP networks are compared with observed MR shown in Figures 3 and 4. These results demonstrate that the agreement is very good in MLP neural network with regard to generalized Page's model, and this model tracks the observed moisture contents well throughout the various conditions (Figure 4).

These models (generalized Page's model, MLP network) were compared based on the R^2, MSE and P, and the results are shown in Table 4. It can be said that the model with lowest MSE or P and highest R^2 was the best model to

Table 1 Training algorithm (LM) for different hidden layers for several networks at threshold function

Threshold function	No. of neurons	MSE	R^2	Threshold function	No. of neurons	MSE	R^2
Tangsig-Tangsig	5	0.000018	0.9987	Tangsig-Purelin	5	0.000078	0.9962
	6	0.000316	0.9936		6	0.000094	0.9965
	7	0.001192	0.9503		7	0.000358	0.9862
	8	0.000044	0.9919		8	0.000081	0.9964
	9	0.001577	0.9053		9	0.000109	0.9616
	10	0.000362	0.9871		10	0.000039	0.9962
	11	0.000316	0.9914		11	0.000149	0.995
	12	0.001573	0.9187		12	0.000268	0.9893
	13	0.000409	0.9805		13	0.000033	0.9969
	14	0.000109	0.9951		14	0.000976	0.9962
	15	0.000800	0.9803		15	0.001000	0.9557
	16	0.002666	0.956		16	0.012897	0.6687
	17	0.000452	0.9392		17	0.000375	0.9833
	18	0.000197	0.9852		18	0.000435	0.9671
	19	0.002185	0.9032		19	0.000543	0.9732
	20	0.002675	0.8883		20	0.000565	0.9585
Purelin-Tangsig	5	0.014014	0.8038	Logsig-Logsig	5	0.006667	0.8223
	6	0.000211	0.965		6	0.003483	0.7611
	7	0.004157	0.8464		7	0.000120	0.989
	8	0.000739	0.9142		8	0.004250	0.8718
	9	0.005879	0.8522		9	0.002530	0.8984
	10	0.000648	0.9365		10	0.000329	0.9699
	11	0.004206	0.7558		11	0.003887	0.8822
	12	0.004018	0.8542		12	0.000115	0.9846
	13	0.004212	0.8153		13	0.011651	0.7829
	14	0.006919	0.8116		14	0.000083	0.9865
	15	0.032522	0.2327		15	0.000374	0.9552
	16	0.000468	0.9571		16	0.003991	0.8018
	17	0.000231	0.9592		17	0.004258	0.8185
	18	0.000885	0.9154		18	0.009275	0.6796
	19	0.004335	0.8574		19	0.007715	0.8645
	20	0.001780	0.8773		20	0.007163	0.667

LM, Levenberg–Marquardt; MSE, mean square error; R^2, coefficient of determination.

Table 2 Statistical results obtained for Page's model

Temperature (°C)	R^2	MSE	P (%)
10	0.999	0.00006	3.3
20	0.999	0.00006	3.1
30	0.993	0.00039	3.8
40	0.996	0.00018	14.3
50	0.996	0.00023	55.3

MSE, mean square error; P, mean relative deviation modulus; R^2, coefficient of determination.

Table 3 Page's model parameters at different soaking conditions of sorghum kernels

Temperature (°C)	k	N
10	0.022	0.606
20	0.041	0.547
30	0.076	0.493
40	0.116	0.466
50	0.079	0.606

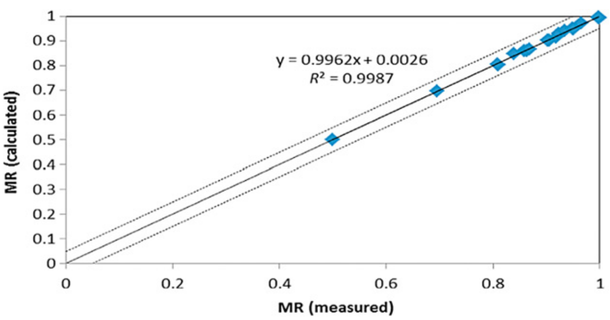

Figure 4 Comparison between measured and calculated values of MR by MLP neural network model. MLP, multilayer perceptron; MR, moisture ratio.

describe the soaking behaviour of sorghum kernel. By this respect, the MLP neural network model with P of 13.34%, and generalized Page's model (P = 24.75%) was selected as the suitable model to describe soaking characteristics of sorghum kernel.

Table 4 Statistical results obtained for generalized Page's model and MLP network

Model	R^2	MSE	P (%)
Page	0.983	0.00070	24.70
MLP	0.998	0.00001	13.34

MLP, multilayer perceptron; MSE, mean square error; P, mean relative deviation modulus; R^2, coefficient of determination.

Conclusion

Based on this study, the following conclusions can be stated:

(1) The soaking temperature had great effect on the soaking kinetics of sorghum kernel.
(2) The water adsorption increased when the soaking temperature increased from 10 °C to 50 °C, and the soaking time decreased with increase in soaking temperature.
(3) The Page's model with the generalized k and N fitted the soaking data of the sorghum kernel with high R^2 and low MSE and *P* values.
(4) The best model to describe the soaking characteristics of sorghum kernel was found to be the MLP neural network with P of 13.34%, followed by and generalized Page's model (P = 24.7%).

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