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Comparison between artificial neural networks and mathematical models for moisture ratio estimation in two varieties of green malt

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Keywords

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Abstract

Introduction Artificial neural network (ANN) 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 a comparison between ANNs and mathematical models for moisture ratio estimation in two varieties of green malt. *Methods* In this study, drying characteristics of two varieties green malt Sahra and Dasht were studied at different temperatures (40, 55, 70 and 85 C) by measuring the decrease in the mass of green malt with respect to time. A feed forward back propagation (FFBP) neural network was used to estimate the moisture ratio of green malt during drying. ANN was used to model green malt drying at different temperatures and a comparison was also made with the results obtained from Page's model. The variety, drying temperature and time were used as input parameters and the moisture ratio was used as output parameter. *Results* The results were compared with experimental data and it was found that the estimated moisture ratio by FFBP neural network is more accurate than Page's model. It was also found that moisture ratio decreased with increasing of drying time and temperature. *Conclusion* The ANN model was more suitable than other models for moisture ratio estimation in green malt.

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Introduction

Drying is the most common food preservation method used in practice (Yaldýz & Ertekýn, 2001; Midilli *et al.*, 2002; Janjai & Tung, 2005) and drying (kilning) of green malt with aim of arrest modification and render malt stable for storage, ensure survival of enzymes for mashing and introduce desirable flavour and colour characteristics and eliminate undesirable flavours have been done (Bamforth, 2005).

The moisture content of green malt is about 42–48% and usually an air temperature ranging from 30 °C to 85 °C or a constant temperature of air may be used to kilning of green malt. High energy cost and the all year round nature of the malting process have led to number of developments in energy conservation. However, the effectiveness of those depends greatly on a theoretical knowledge of the drying process. But a little information about simulation of green malt drying is available.

Artificial neural networks (ANN) 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). Artificial neural networks have already been applied to simulate processes such as fermentation (Latrille *et al*., 1993), cross-flow microfiltration (Dornier *et al*., 1995), drying behaviour of different food and agricultural materials such as carrot (Kerdpiboon *et al*., 2006; Erenturk & Erenturk, 2007; Aghbashloab *et al*., 2011), tomato (Movagharnejad & Nikzad, 2007), cassava and mango (Hernandez-Perez *et al*., 2004) and osmotic dehydration (Fathi *et al*., 2009), but there is no information about application of artificial neural networks in simulation of drying process for green barley malt.

This study was carried out to test and validate the efficiency of ANN for simulating the drying behaviour and the effect of temperature and time on the drying of green barley malt. The results were also compared with those obtained from Page's model.

Mathematical models are the most common methods for the estimation of moisture ratio (MR). These models, which are fitted to experimental data, have many problems, such as reduction of computation velocity and accuracy of processing control systems as well as production of numerous equations. The development of a deep-bed drying simulation model is a valuable tool for optimization of design and prediction of performance of the drying system for germinated barley (malt kilning). Thin-layer drying models are required for simulation of deep-bed drying of germinated barley, hereafter referred to as 'malt'. Simulation models provide an opportunity for the assessment of the energy conservation and saving alternative without full-scale experiment (Bala & Woods, 1992).

Upon the mathematical model or ANNs determination through their programming into a control system, it could be possible to predict MR. For that, the main objective of this research was to select the best method for predicting drying, in order to use them for the calculation of drying time and energy consumption.

Materials and methods

Preparation of green malt

In this study, two most important varieties of barley for malting in Iran, Sahra and Dasht, were used. These varieties were obtained from the Seed and Plant breeding Institute of Jahad-Agricultural Organization, Gonbad, Iran. The samples were manually cleaned to remove foreign matter, dust, dirt, broken and immature grains.

To produce malt, cleaned barley varieties were steeped to raise the water content from 9–11% to around 45% at 17 °C. This process takes about 48 h. The moist grains were then allowed to germinate at 17 °C for 6–7 days, then the 'green malt' is ready for kilning.

Experimental apparatus

Drying experiments were performed at the Department of Food Science and Technology of Gorgan University of Agricultural Sciences and Natural Resources. An electric thermal blast dryer [Type WB-OB7- 45, Memmert (small East Frisian island of the northern coast), Germany] was used for drying germinated barley, which could be regulated to any desired drying air temperature between 30 °C and 200 °C with high accuracy. A balance with an accuracy of 0.001 g was used to measure the weight of the samples. The air velocity in the tubes just before the trays was 6 m s^{-1}.

Experiments were performed at air temperatures of 40, 55, 70 and 85 °C. At least three repetitions were done for each drying temperatures. For the drying experiments the trays were loaded with 200 g green malt to have similar airflow resistance. During the drying process, the weight of the samples was measured by taking the trays out of the dryer. The shorter time intervals for weighing have been chosen at the beginning of each test than at the end. For instance, the time interval was 15 min at the first 5 h of drying and 30 min later. All the tests were continued to reach to a constant weight of the samples. After drying, the final Moisture content (M) of the samples was measured using the oven method (105 °C, 24 h). The final dry matter mass of a sample was used to derive the temporal course of M during the drying experiment:

$$M_t = \frac{W_t - DM}{DM}, \tag{1}$$

in which M_t is the moisture content in decimal during the drying process at time t, W_t is the weight of the sample in kg at time t and DM is the dry matter weight in kg. As a check, also, the initial M of the fresh sample was measured before each drying test.

Mathematical drying isotherm models

For calculating M_e at each air temperature, the specified sample placed in dryer and kilning were continued to reach to a constant weight. Then M_e was calculated from previous equation.

The MR of the green malt during the drying experiments was calculated using the following equation:

$$\mathrm{MR} = \frac{M_t - M_e}{M_0 - M_e}, \tag{2}$$

in which M_t is moisture content (dry basis) at time t, M_e is equilibrium moisture content and M_0 is initial moisture content.

Table 1 Some of mathematical equations given by various authors for the drying curves and grouping of the equation based on the mathematical similarity

No.	Model name	Equation	Coefficients	Reference
1	Lewis	$MR = \exp(-kt)$	1	Lewis (1921)
2	Henderson and pabis	$MR = a \exp(-kt)$	2	Henderson & Pabis (1961)
3	Page	$MR = \exp(-kt^n)$	2	Page (1949)
4	Modified page	$MR = \exp(-kt)^n$	2	Overhults *et al*. (1973), White *et al*. (1981)
5	Two-term	$MR = a \exp(-k_1 t) + b \exp(-k_2 t)$	4	Henderson (1974), Yaldýz & Ertekýn (2001)
0	Wang and Singh	$MR = 1 + at + bt^2$	Rejected	Wang & Singh (1978)
0	Midilli and Kucuk	$MR = a \exp(-kt^n) + bt$	Rejected	Midilli *et al*. (2002)

The most common physical models for drying of agricultural products include the models was made based on the literature (Table 1).

All equations are monotonic decreasing equations, which is the property of drying, except the Wang and Singh, and Midilli and Kucuk equations. The Wang and Singh equation as well as Midilli and Kucuk equation are rejected because these equations may lead to an increase of MR at the long term.

The remaining equations were arranged in the order of complexity. The complexity was defined based on number of coefficients, number of terms and power of time. For instance, the Lewis equation, which is the simplest among the equations, has one coefficient, one term and the power of time is one. The equation of two terms has four coefficients and the power of *t* is one. Finally, we can conclude that there are five different equations for fitting to the data (Table 1).

The moisture content data obtained at different drying air temperatures were converted to the MR. Then, the selected MR equations were fitted to the experimental data of green malt that produced from two variety of barley separately.

The fitting steps for both variety of green malt were as follows:

(1) A linear regression program in MATLAB 7.10 software, with the Neural Network Toolbox 4 (The Mathworks, Inc., Natick, MA, USA) was used to fit the equations to the experimental data to find the equation and the error parameters coefficient of determination (R^2; Saeed *et al*., 2008) and the least mean square error (MSE; Iguaz *et al*., 2003) and mean relative deviation (MRD; Sun, 1999).
(2) The best equation was selected based on the higher values for R^2 and the lower values for MSE and MRD and simplicity (less parameter).
(3) The parameters in the equations were fitted as a function of temperature.

Artificial neural network

Artificial neural network 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). An ANN consists of neurons, which have been related with special arrangement. Neurons are in layers and every network includes some neurons in input layer, one or more neurons in output layer and neurons in one or more hidden layers. Algorithms and architectures of artificial neural networks are different through variation in neuron model and relationship between neurons, and their weights. The learning purpose in ANNs is weights updating, so that with presenting set of inputs, desired outputs are obtained. The most common types of ANNs include feed forward, feedback and competitive (Menhaj, 1998; Jam & Fanelli, 2000). Training is a process that finally results in learning. Each network is trained with presented patterns. During this process, the connection weights between layers are changed until the differences between predicted values and the target (experimental) is reduced to the permissible limit. Weights interpret the memory and knowledge of network. With the aforementioned conditions, learning process take place. Trained ANN can be used for prediction of outputs of new unknown patterns (Heristev, 1998). The advantages of using ANN are high computation rate, learning ability through pattern presentation, prediction of unknown pattern and flexibility affront the noisy patterns. In this research, feed forward network was utilized.

Feed forward back propagation (FFBP) consists of one input layer, one or several hidden layers and one output layer. For learning this network, back propagation (BP) learning algorithm is usually used. In the case of BP algorithm, the first output layer weights were updated. A desired value exists for each neuron of output layer. The weight coefficient was updated by this value and learning rules. BP algorithm presents suit results for subsequent problems but for the other problems gives an improper result. In some cases, the learning process was upset due to local minimum. This happens because of laying the answer at the smooth part of threshold function.

During training this network, calculations were carried out from input of network towards output and values of error were then propagated to prior layers. Output calculations were conducted layer to layer so that the output of each layer was the input of next one.

Levenberg-Marquardt (LM) training algorithm was used for updating network weights. Gradient-based training algorithms, such as back propagation, are most commonly used by researchers. They are not efficient because the gradient vanishes at the solution. Hessian-based algorithms allow the network to learn features of a complicated mapping more suitable. The training process converges quickly, as the solution is approached because the Hessian does not vanish at the solution. To benefit the advantages of Hessian-based training, LM algorithm was used. The LM algorithm is a Hessian-based algorithm for non-linear least squares optimization (Hagan & Menhaj, 1994).

Structural learning with forgetting is the main technique used for regularization (Girosi *et al*., 1995; Kozma *et al*., 1996). It has a good approximation with arbitrary accuracy of training and can also improve generalization performance.

Designing the ANNs

Considering and applying the three inputs in all experiments, the MR value derived for different conditions. Networks with three neurons in input layer (variety, temperature and time) and one neuron in output layer (MR) were designed. Figure 1 shows the considered neural

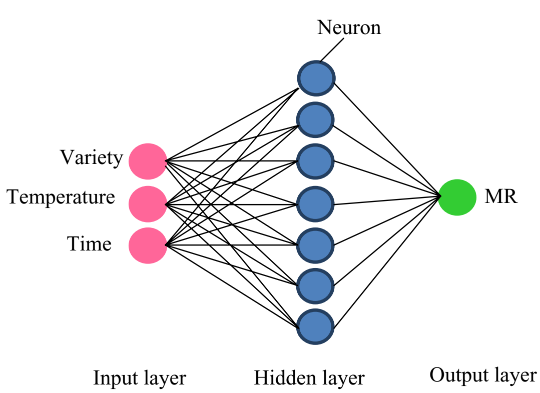

Figure 1 Feed forward back propagation neural network.

network topology and input and output parameters. Boundaries and levels of input parameters are shown in Table 2. In addition, two variety of Sahra and Dasht had used. Neural network toolbox (ver. 7.10) of MATLAB software was used in this study.

Two important factors must be considered in order to ensure a successful modelling of FFBP. First, is the number of hidden layers and second is the number of neurons in each hidden layer. Since almost all of the problems in neural network modelling could be solved with one hidden layer (Chen *et al*., 2001; Mohebbi *et al*., 2007; Movagharnejad & Nikzad, 2007; Ochoa-Martínez *et al*., 2007; Kashaninejad *et al*., 2008; Mitra *et al*., 2011), an ANN with one hidden layer was used in this research. In addition, using too many hidden layers may lead to problem of data over fitting, affecting the system's generalization capability (Abdullah *et al*., 2006). On the other hand, to find the best architecture, different networks were built with different hidden neurons varying from 7 to 20.

Training process by FFBP network is iterative. When the error between desired and predicted values is minimum, training process meets the stability. The increasing method was used for selection layers and neurons for evaluation of various topologies. By this method, when the network is trapped into the local minimum, new neurons are gradually added to the network.

This method has more practical potential to detect the optimum size of the network. The increasing method has some advantages which are (a) the network complexity gradually increases with increasing neurons; (b) the optimum size of the network always obtains by adjustments; and (c) monitoring and evaluation of local minimum carry out during the training process. Various threshold functions were used to reach the optimized status (Demuth & Beale, 2003):

$$Y_j = \frac{1}{1+\exp(-X_j)} \text{(LOGSIG)} \tag{3}$$

$$Y_j = \frac{2}{1+\exp(-2X_j)-1} \text{(TANSIG)} \tag{4}$$

$$Y_j = X_j \text{(PURELIN)} \tag{5}$$

Table 2 Input parameters for ANNs and their boundaries

Parameters	Minimum	Maximum	No. of levels
Air temperature(°C)	40	85	4
Time (min)	0	600	31

In which X_j is the sum of weighed inputs for each neuron in j^{th} layer and computed as below:

$$X_j = \sum_{i=1}^{m} W_{ij} \cdot Y_i + b_j \tag{6}$$

where m is the number of output layer neurons, W_{ij} the weight of between i^{th} and j^{th} layers, Y_i the i^{th} neuron output and b_j, bias of j^{th} neuron for FFBP network. About 70% of all data were selected for training network with suitable topology and training algorithm.

The following criterion of root MSE has defined to minimize the training error (Demuth & Beale, 2003):

$$MSE = \sum_{p=1}^{M} \sum_{i=1}^{N} \left(S_{ip} - S_{ip}\right)^2 \tag{7}$$

where MSE is the mean square error, S_{ip} the network output in i^{th} neuron and p^{th} pattern, T_{ip} the target output at i^{th} neuron and p^{th} pattern, N the number of output neurons and M the number of training patterns. To optimize the selected network from prior stage, the secondary criteria were used as follow:

$$R^2 = 1 - \frac{\sum_{k=1}^{n} [S_k - T_k]}{\sum_{k=1}^{n} \left[S_k - \frac{\sum_{k=1}^{n} S_k}{n} \right]} \tag{8}$$

Where R^2 is the determination coefficient, error, S_k the network output for k^{th} pattern, T_k the target output for k^{th} pattern and n the number of training patterns. To increase the accuracy and processing velocity of network, input data was normalized at boundary of [0, 1].

Results and discussion

Experimental results

Figure 2 presents the drying curves of the Dasht and Sahra green malts, which were dried at the same air temperature (40 °C). They showed almost a similar behaviour.

Drying curves determined that drying of green malts of two varieties occurs in the falling rate period. To describe this phenomenon, the drying rate was calculated at different times and temperatures and plotted against moisture content (d.b. %) as shown in Figure 3. Initially, the drying rate was higher because of initially water for evaporation comes from regions near the surface. As drying progressed, the drying rate decreased with decrease of moisture content, as the water to be evaporated comes from parenchyma cells within the structure and must be transported to the surface. The falling rate region is indicative of an increased resistance to both heat and mass transfer through the inner cells.

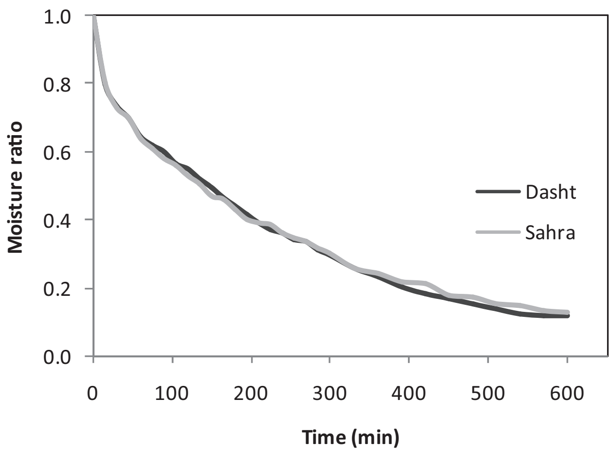

Figure 2 Moisture ratio changes of Sahra and Dasht green malts at 40°C.

Selection of the best mathematical equation

All the data series were fitted to the remaining five equations.

The average values of the R^2, MSE and MRD for all equations at different temperature are shown in Figure 4 for Sahra and Dasht green malts. The higher value of R^2 and lower value of, MSE or MRD shows a higher accuracy of the fitting. In Figure 4, Lewis and Henderson and Pabis models have low values of R^2 and high values of MSE and MRD. Although the Page, Modified Page and two-term were very similar among the selected equations, the Page equation was selected as the appropriate equation for this research because the levels of the Page equation were very similar, but the Page equation is simpler with two parameters while the two-term equation has four parameters. The lower numbers of parameters is preferable to find a relationship between the parameter values and the drying conditions. Also, the Page equation is simpler than the Modified Page.

The experimental data were fitted to the Page equation to find the K and N-values simultaneously at each temperature. For the N-value at different temperatures, a polynomial equation was fitted for Sahra as well as Dasht green malts using all data series. The results are given in Eq. 9 for Sahra (S) and Eq. 10 for Dasht green malts (D), T represents the temperature in °C

$$N_S = \left(-6 \cdot 10^{-5} T^2\right) + (0.0099T) + 0.3773 \tag{9}$$

$$N_D = \left(-0.0004T^2\right) + (0.043T) - 0.4496 \tag{10}$$

Several expressions were applied for the relation of K and temperature. The exponential and polynomial equations were chosen to find the best fit for the k-values as a function

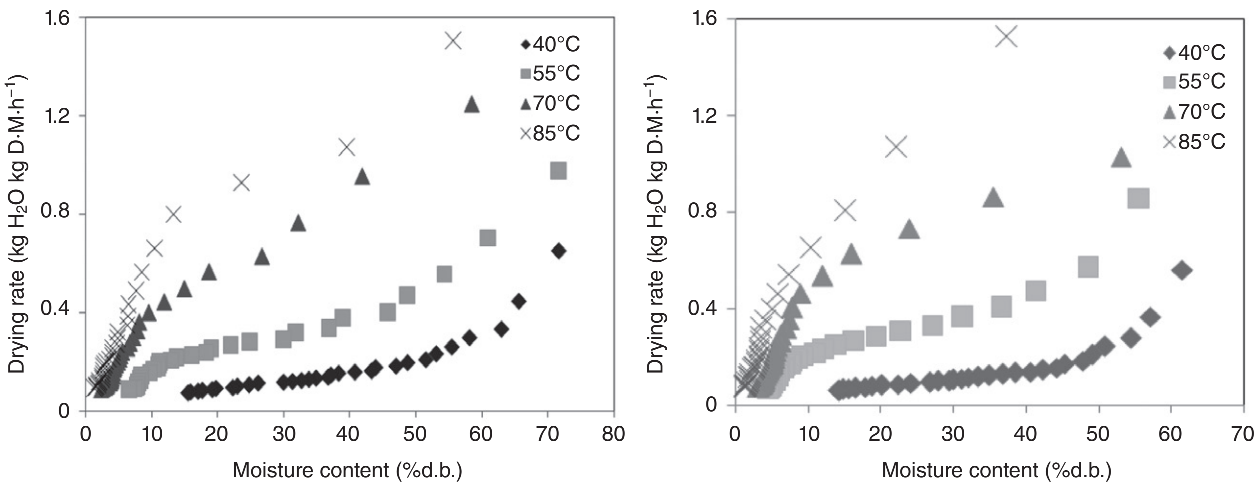

Figure 3 Effect of temperature on drying rate of Sahra and D green malt (respectively from left to right).

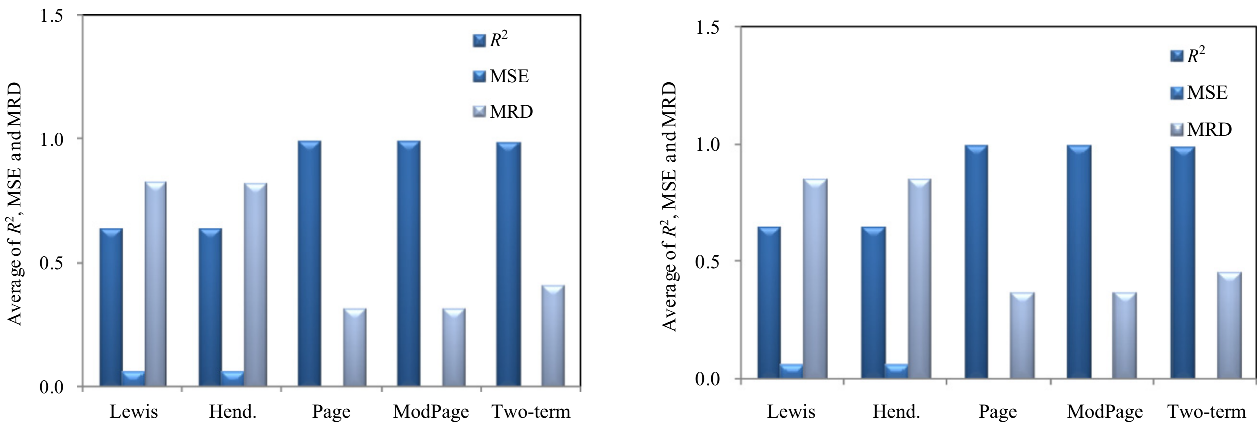

Figure 4 The average level of R^2, MSE and MRD of all data series for different drying equations for Sahra and D green malt (respectively from right to left).

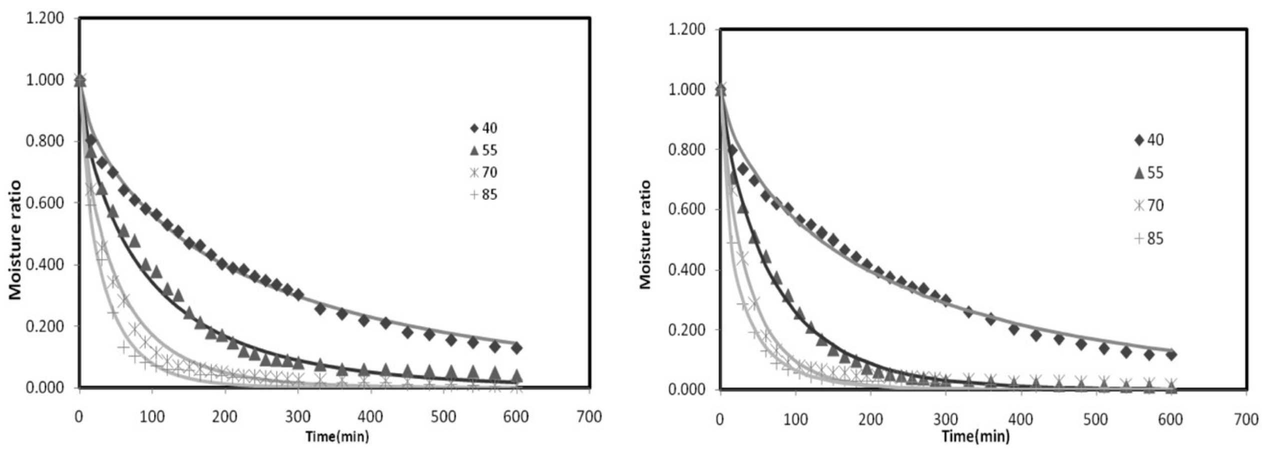

Figure 5 Effect of temperature on drying rate of Sahra and D green malt (respectively from right to left).

Table 3 Training algorithm for different neurons at one hidden layer for several networks at the threshold function for layers

Network	Training algorithm	Threshold function	No. of neurons	MSE	R^2
FFBP	LM	TANSIG-PURELIN	8	0.0006	0.937
			10	0.0004	0.954
			12	0.0008	0.920
			14	0.0000	0.997
			16	0.0002	0.978
			18	0.0005	0.946
			20	0.0005	0.947
FFBP	LM	LOGSIG-PURELIN	8	0.0606	0.934
			10	0.0606	0.991
			12	0.0636	0.817
			14	0.0607	0.802
			16	0.0603	0.977
			18	0.0607	0.940
			20	0.0601	0.989

of temperature (T in °C) for Sahra and Dasht green malts, respectively. Finally, the following equations were found for drying of those:

$$K_S = 0.0106\exp^{(0.0219T)} \tag{11}$$

$$K_D = (8 \cdot 10^{-5} T^2) - (0.0078T) + 0.2071 \tag{12}$$

The complete equation become therefore for Sahra Eq. 13, and for Dasht green malt Eq. 14.

$$MR_S = \exp\left(-\left(0.0106\exp^{(0.0219T)}\right)t^{\left(-6\cdot10^{-5}T^2\right)+(0.0099T)+0.3773}\right) \tag{13}$$

$$MR_D = \exp(-((8\cdot10^{-5}T^2) - (0.0078T) + 0.2071)t^{(-0.0004T^2)+(0.043T)-0.4496}) \tag{14}$$

Some of the experimental MR values as a function of time are presented in Figure 5 for Sahra and Dasht green malt together with the predicted values using the above given exponential equations. We can see that these equations are good enough to estimate the M at different drying time for our purpose of calculating energy and drying time.

ANNs approach

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 (Table 3). This strategy, together with learning algorithm of LM, was used for FFBP networks. Several topologies were tested and the best results, which were used from each network, training algorithm and threshold functions, are represented in Table 4.

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

Model	R^2	MSE	Average (c m^{-1})[1]	SD (c m^{-1})
Generalized page	0.985	0.00016	0.98	0.02
FFBP	0.997	0.00003	1.00	0.01

[1]c m^{-1}, proportion of calculated to measured.

With regard to the results, the strategy of FFBP network, LM algorithm with TANSIG-PURELIN threshold functions and 14 neurons showed the best performance. This is because MSE and R^2 have the better values.

A comparison of drying curves based on the experimental data and the optimum ANN topology for all drying air temperature of and different varieties is shown in Figure 6. The optimal ANN model provided good agreement between experimental and predicted MR, which indicates the suitability of the proposed ANN model to describe the drying behaviour of green malt.

Comparison between mathematical model and ANN

MR predicted with the generalized Page's model and FFBP network are compared to the observed MR in Figures 7 and 8. In these figures, the dotted lines represent the 0.95 and 1.05 measured data. These results demonstrate that the agreement is very good in FFBP neural network and this model tracks the observed moisture contents well throughout the various conditions.

These models (generalized Page's model and FFBP network) were compared based on the coefficient of determination (R^2), MSE and the results about average and standard deviation (SD) of proportion of calculated to measured (c m^{-1}) are shown in Table 4. It is assumed that the model with lowest MSE or SD (c m^{-1}), highest R^2 and closer to one average (c m^{-1}) is the best to describe drying behaviour. Therefore, the suitable model to describe drying characteristics of green malt was found to be the FFBP neural network with $R^2 = 0.997$, MSE = 0.00003, average (c m^{-1}) = 1.00 and SD(c m^{-1}) = 0.01.

Conclusions

As the drying behaviour of the Sahra and Dasht green malts was similar, the same drying model can be used for both varieties.

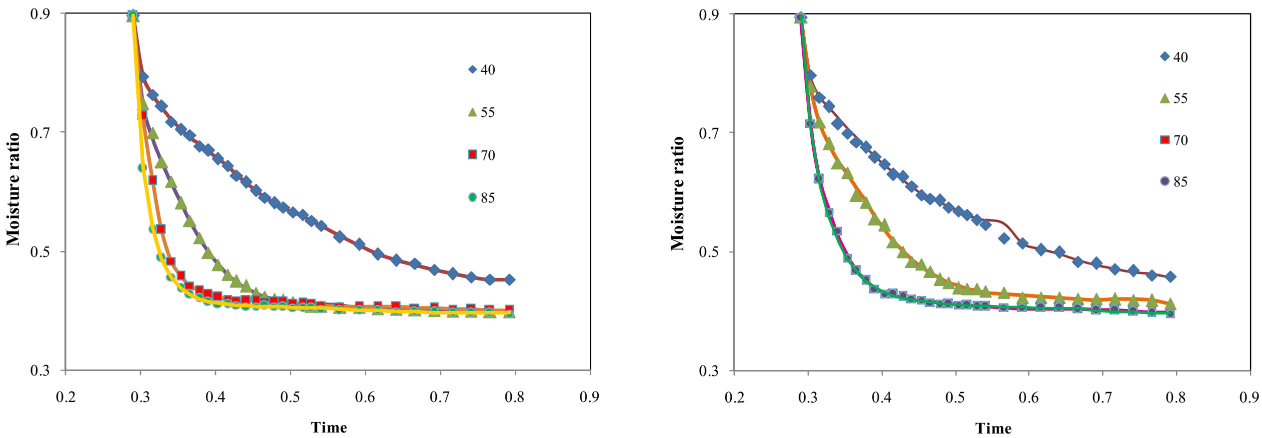

Figure 6 Experimental and predicted moisture ratio for Sahra and D using optimum ANN model (respectively from right to left).

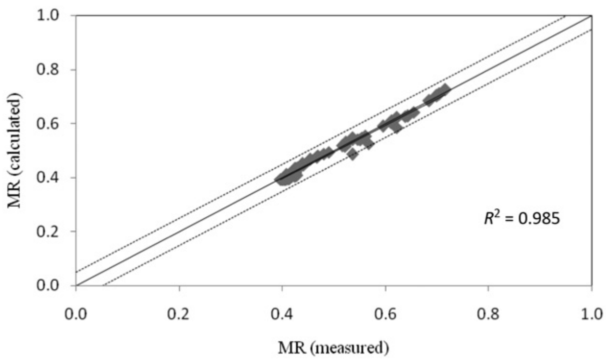

Figure 7 Comparison between measured and calculated values of MR by generalized Page's model.

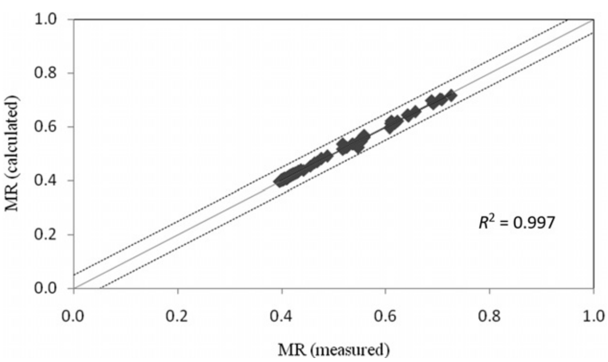

Figure 8 Comparison between measured and calculated values of MR by FFBP neural network model.

Among the drying equations, which were evaluated in this research, the Page, Modified Page and two-term equations showed the similar fit. The difference between the Page equation and the two-term equation is small. The Page equation is simpler than Modified Page and that has two variables, which makes it easier to find the dependency of the parameters with temperature. Therefore, the Page equation is a mathematical model selected as a relevant equation for drying of green malt.

Relevant equations as well as *N* and *K*-values were found as function of temperature for Sahra and Dasht green malts. Equations show small differences with experiments. The equations can be used at temperatures 40–85 °C. They are suitable to estimate the moisture content during drying in order to calculate energy consumption, drying time and cost estimations. They are also usable in dryer design.

The FFBP neural network was the best model to describe the drying characteristics of green malt with average (c m^{-1}) = 1, followed by generalized Page's model for Sahra and Dasht varieties [average (c m^{-1}) = 0.98].

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