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Comparison between mathematical models and artificial neural networks for prediction of sorption isotherm in rough rice

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A b s t r a c t. Equilibrium moisture content data for long grain rough rice (*Oryza Sativa*, cv. Binam) were obtained by equilibrating rough rice samples at different equilibrium relative humidity (*ERH*) and temperatures. Although conventional mathematical models are able to predict *EMC* with high accuracy, such models can be competed and replaced with artificial neural networks (ANNs) method which is a simple mathematical model of human brain performance. Modified models of Chung-Pfost, Halsey, Henderson, Oswin as well as GAB were used as mathematical models to fit the data. One of the multi layer perceptron (MLP) neural network types, called Feed Forward Back Propagation (FFBP), was used in this work. Training algorithm of Levenberg-Marquardt (LM) was also applied. The range of temperature was 0-35 with 5°C intervals and relative humidity was 19.75-94.21%. The best results for mathematical model belonged to the Chung-Pfost model with average R^2 = 0.9861 and mean relative error = 4.76%, and the best one for FFBP neural network with training algorithm of LM was appertained to the topology of 2-4-3-1 and threshold functions order of TANSIG-TANSIG-PURELIN. By the use of this optimized network, R^2 = 0.9958 and mean relative error = 3.56% were determined. These results show that mathematical models can be replaced with the ANNs for the prediction of *EMC* in the Binam variety of rough rice.

K e y w o r d s: rough rice, sorption isotherm, equilibrium moisture content , mathematical models, artificial neural network

INTRODUCTION

Rice is one of the most important foods for the majority of the people in the world. Manual control of rice processing systems can decrease the ultimate quality of rice, thus intelligent control of processing systems can prevent it. Some investigations on the moisture content changes of stored rice with air temperature at the duration of aeration have been carried out for different cultivars using models with three or more coefficients represented (Jindal and Siebenmorgen, 1994).

Rough rice has a hygroscopic nature and ventilation of a bin to reduce rough rice temperature can cause rough rice to gain or lose moisture, depending on the rough rice-air interactions that take place. An equation that relates the equilibrium relative humidity (*ERH*) to the grain equilibrium moisture content (*EMC*) is needed to optimise the grain quality. Rice is a very delicate cereal and difficult to manage. Because it is consumed as whole kernel, the formation of fissures and cracking provoked through ventilating with high air relative humidity negatively affects its final quality (Siebenmorgen *et al*., 1998). Several investigators have studied the sorption model of cereals (Chen and Jayas, 1998; Sokhansanj and Yang, 1996). Many researchers investigated the relation of *EMC* changes of stored rice with air temperature, air flow rate during aeration, and variety (Khankari *et al*., 1994).

Equilibrium moisture content of some foods and agricultural products has been investigated by many researchers: sugar beet root (Iglesias *et al*., 1975), potato slices (Mazza, 1982), rough rice (Aguerre *et al*., 1983), shelled maize (whole, dehulled and hulls) (Tolaba and Suarez, 1990), mustard seeds (Mazza *et al*., 1994), extruded rice-legume snacks (Chauhan and Bains, 1990), starch gels (McMinn *et al*., 2004), almond (Pahlevanzadeh and Yazdani, 2005), mushroom (Lee and Lee, 2008) and olive leaves (Bahloul *et al*., 2008). Artificial neural networks have been used in some industrial applications such as: performance prediction of an industrial paper dryer (Huang and Mujumdar, 1995), predictive control of a drying process (Jay and Oliver, 1996), modelling the moisture content of thin layer corn during drying process (Trelea *et al*., 1997), air heater plant for a dryer (Thyagurajan *et al*., 1997) and sorption isotherm of black tea (Pancharyia *et al*., 2002).

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The relationship between *EMC* and *ERH* is of a crucial importance in heat and mass balances. Its knowledge permits the optimisation of the energetic efficiency of drying installations and of product quality during storage ventilation, which represents an important step forward for the rice industry. Equilibrium moisture characteristics have a very important role in post harvest stages. Many researchers have worked on equilibrium moisture content of foods and agricultural products. The most common method for estimation of equilibrium moisture content is mathematical models. Application of models which are fitted to experimental data involves many difficulties, such as the generation of numerous equations, reduction of computation velocity and reduction of accuracy of processing control systems. Precise prediction of *EMC* can not only decrease the storage losses of rough rice, but it may also affect the processing systems. Determining a mathematical model or ANNs, and programming it into a control system, would make it possible to predict the *EMC* irrespective of whether aeration causes the drying or wetting of the mass of rice at a safe level.

Mathematical models with three or more coefficients would fit the empirical data better, but the use of an additional coefficient must introduce significance in improving the goodness of fit. Relationship between *EMC* and *ERH* varies among rice cultivars. No data regarding adsorption were found for the Binam rice cultivar.

The propose of the present work was to:
– study at temperatures simulating the local climatic conditions of the Guilan province (Iran) by mathematical models,
– create a relation between equilibrium moisture content, equilibrium relative humidity and ambient temperature using an artificial neural networks,
– compare the results of the two methods.

MATERIAL AND METHODS

The long grain rough rice of Binam cultivar (average length of 7 mm) was supplied by a rice processing factory in Astane city, Guilan province, Iran, after first drying in a drying bin (August, 2006). According to the local synoptic station, the average monthly maximum temperature and relative humidity of this region were 29°C and 95%, respectively. The average moisture content of rough rice, based on random bulk sampling, was about 17±1% (d.b.) (Zomorodian, 2001). The adsorption isotherms were determined by the static method with different sulphuric acid solutions (Merk, Germany) to achieve the internal *ERH* in jars (Iglesias and Chirife, 1982; Molnar, 1995). A sulphuric acid volume of 125 ml was introduced into jars, with concentrations varying between 10 to 58% (w/w). *ERH* or water activity (a_w) for every temperature was determined using the Molnar equation (Molnar, 1995). Rice samples were dried in a laboratory dryer (made at the Department of Agricultural Machinery Engineering, Bu-Ali Sina University, Hamedan, Iran) at 70°C and pressure less than 100 mm Hg (AOAC, 1990), then 2-3 g of dried rice were introduced in a small basket and suspended from the jar lid above the solutions. The jars were placed in temperature control apparatus (Lutron TM-915, Taiwan) from 0 to 35 at 5°C intervals. Nine points were obtained to determine the adsorption isotherm. Each experiment was done in three replications. The time needed for the samples to reach equilibrium varied from 2 to 8 weeks, depending on the temperature of the experiment. Moisture content of samples was determined by using the gravimetric method with a balance type GF-600 (± 0.001), AND, Japan.

Five most common physical models for deriving *EMC* of agricultural products are modified models of Chung-Pfost, Halsey, Henderson, Oswin as well as GAB. These models have been proposed and tested for the dependence between *EMC* and water activity (Garcia-Alvarado *et al*., 1995; San Martin *et al*., 2001; Sanny *et al*., 1997). The formula of each model is as follows:

$$EMC = \frac{1}{\mathrm{B}}\left[\left(\ln \frac{\mathrm{A}}{\mathrm{R}(T+\mathrm{C})}\right) - \ln\left(-\ln a_w\right)\right] \tag{1}$$

(Modified Chung-Pfost),

$$EMC = \frac{\mathrm{ABC}a_w}{\left(1-\mathrm{C}_{a_w}\right)\left[\left(1+(\mathrm{B}-1)\mathrm{C}_{a_w}\right)\right]} \tag{2}$$

(GAB),

$$EMC = \left[\frac{-\exp(\mathrm{A}+\mathrm{B}T)}{\ln a_w}\right] \tag{3}$$

(Modified Halsey),

$$EMC = \left[-\frac{1}{\mathrm{A}(T+\mathrm{C})}\ln\left(1-a_w\right)\right]^{\frac{1}{\mathrm{B}}} 10^{-2} \tag{4}$$

(Modified Henderson),

$$EMC = \left(\mathrm{A}+\mathrm{B}T\right)\left(\frac{a_w}{1-a_w}\right)^{\frac{1}{\mathrm{C}}} \tag{5}$$

(Modified Oswin),

where: a_w is water activity, *EMC* is equilibrium moisture content (% d.b.), T is absolute temperature (K), R is universal gas constant (8.314 J mol^{-1}K^{-1}), A, B, and C are constants for different materials that were calculated by experimental method. Supremacy of each model for prediction of *EMC* was expressed by two indices of coefficient of determination (R^2) and mean relative error (E_{mr}). The fit was performed by non-linear regression based on minimization of the square sum by means of the software Statgraphics plus 4.1.

An artificial neural network consists of neurons which have been related together with special arrangement. Neurons are in layers and every network consists of some neurons in input layer, one or more neurons in output layer, and neurons in one or more hidden layers. The learning purpose in artificial neural networks is weights updating, so that with presenting set of inputs, desired outputs are obtained. The most common type of artificial neural networks is Feed Forward Back Propagation (FFBP) (Jam and Fanelli, 2000). 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) are reduced to reach permissible limit (Heristev, 1998). An epoch is the number of sets of training data presented to the network (learning cycles) between weight updates. It is useful to set an epoch, since certain instruments (such as RMS error graph) update their calculations at the end of an epoch.

FFBP network consists of one input layer, one or several hidden layers and one output layer. For learning this network, a back propagation (BP) learning algorithm is usually used. In the case of BP algorithm, first output layer weights are updated. A desired value exists for each neuron of output layer. By this value and learning rules, the weight coefficient is updated.

The Levenberg-Marquardt (LM) training algorithm was used for updating network weights. The LM algorithm is Hessian-based and allows the network to learn features of a complicated mapping more easily. The training process converges quickly as the solution is approached, because the Hessian does not vanish at the solution (Demuth and Beale, 2003).

Considering two inputs in all experiments, the *EMC* value was derived for different conditions. The equilibrium relative humidity (*ERH*) and environmental air temperature affect the Equilibrium Moisture Content (*EMC*) of rice, so *EMC*=f (*ERH*, T), therefore, networks with two neurons in the input layer (*ERH* or water activity and temperature) and one neuron in the output layer (*EMC*) were designed. Boundaries and levels of input parameters are shown in Table 1. Neural network toolbox (ver. 4.1) of MATLAB software (Mathworks Co., USA) was used in this research project.

For obtaining the desired answer, an FFBP network was utilised. During training of this network, calculations were done from input of network toward output, and then values of error propagated to prior layers. Output calculations were done layer to layer and output of each layer was the input of next layer. Various threshold functions were used to obtain the optimized status (Demuth and Beale, 2003): LOGSIG, TANSIG and PURELIN.

About 75% of all data were randomly selected for training network with suitable topology and training algorithm.

T a b l e 1. Input parameters for ANNs and their boundaries

Parameters	Minimum	Maximum	No. levels
Air temperature (°C)	0	35	8
Relative humidity (%)	0.1975	94.21	9

The following criterion of root mean square error was defined to minimise the training error:

$$\mathrm{MSE} = \sum_{p=1}^{M} \sum_{i=1}^{N} \left(S_{ip} - T_{ip} \right)^2 , \tag{6}$$

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

$$R^2 = \frac{\sum_{k=1}^{n} \left[S_k - T_k \right]}{\sum_{k=1}^{n} \left[S_k - T_m \right]} , \qquad \left(T_m = \frac{\sum_{k=1}^{n} S_k}{n} \right) \tag{7}$$

$$E_{mr} = \frac{100}{n} \sum_{k=1}^{n} \left| \frac{S_k - T_k}{T_k} \right| , \tag{8}$$

where: R^2 is coefficient of determination, E_{mr} is mean relative error, S_k is network output for k-th pattern, T_k is target output for k-th pattern and n is the number of training patterns. For increasing the accuracy and processing velocity of network, input data were normalized at boundary of [0, 1].

RESULTS AND DISCUSSION

Results of five mathematical models are shown in Table 2. Coefficients and indices show that two models – modified Chung-Pfost and modified Henderson – gave the best results, because these models presented the best values of MSE, R^2, and E_{mr}. On the other hand, the modified Chung-Pfost and modified Henderson equations better fitted the experimental data including the temperature effect. Modified Oswin and modified Halsey models gave the lowest R^2 and the highest E_{mr} so they were incapable of explaining the variability of the data. The modified Chung-Pfost presented the best results, because its R^2 and E_{mr} were the best values (0.9861 and 4.76, respectively). The GAB equation showed a high error value. In addition, the parameter A which represents the mono-layer moisture content was considerably higher than the data reported in the literature (Chen and Jayas, 1998) and indicated disability of this model to fit the data.

Increase in temperature produces a decrease in *EMC* of rice (Fig. 1). *ERH* at 0.6 and 0.8 determined a 5.55% *EMC* variation at 15 °C. For a constant *ERH* line, the variation of *EMC* was 1.13% at the studied temperature range. Moreover, the distance between constant *ERH* lines was not proportional, indicating that the higher the *ERH*, the higher the water retention capacity of rice. The risk area, where moulds develop due to the high *ERH*, starts at about 80% which is the growth limit for the majority of moulds (Caurie, 2007),

T a b l e 2. Coefficients of the models used to fit the experimental data and the analytical indices

Parameter	Modified Chung-Pfost	Modified Henderson	GAB	Modified Halsey	Modified Oswin
A	4313.25	0.0001	0.1075	-5.13	0.1125
B	14.75	1.30	0.3244 exp (466.61/(273+T))	0.00158	-0.0000857
C	-80.92	118.56	0.7449	2.164	2.48
E_{mr} (%)	4.76	4.97	9.62	11.73	8.73
R^2	0.9861	0.9852	0.9820	0.9380	0.9611

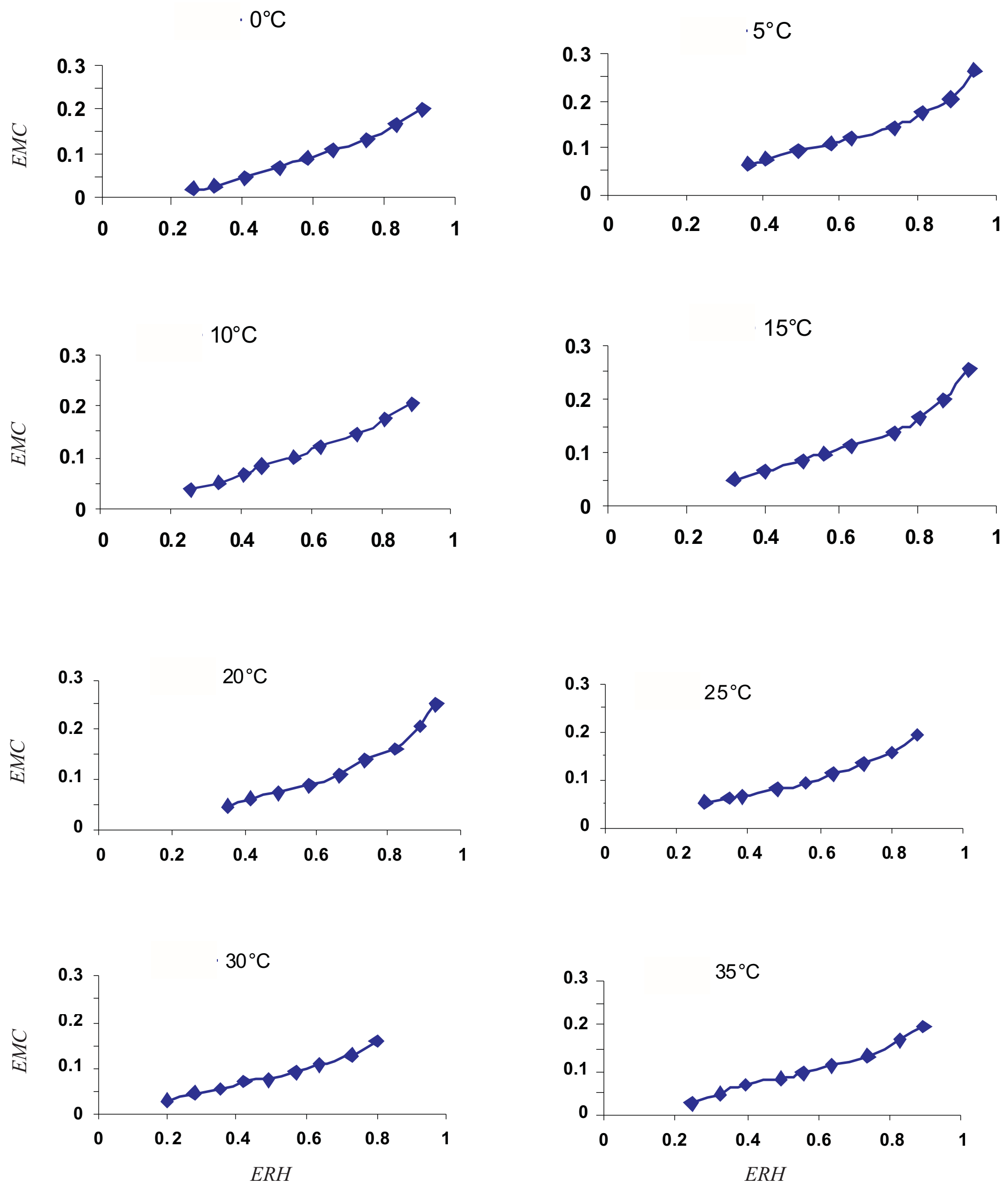

Fig. 1. Mean *EMC* of rice for temperatures between 0-35°C and *ERH* between 0.2-0.93.

T a b l e 3. Best results of applied topologies and threshold functions for FFBP network and LM algorithm

Threshold function	No. layers and neurons	MSE	R^2	E_{mr} (%)	Epoch*
TANSIG	2-4-1	0.0000287	0.9895	5.96	30
LOGSIG	2-5-1	0.0000226	0.9903	5.50	25
TANSIG	2-4-4-1	0.0000235	0.9886	6.07	41
LOGSIG	2-4-3-1	0.0000180	0.9930	4.08	20
TANSIG- TANSIG- PURELIN	2-4-3-1	0.0000153	0.9958	3.56	53

*Number of training cycles.

which coincides with a 16% *EMC*. In general terms, to achieve good storage, the grain mass should have moisture content lower than 16% (d.b.) at a temperature lower than 10°C (Aguerre *et al*., 1983; Siebenmorgen *et al*., 1998). For instance, air at 5°C and 72% RH would equilibrate the Binam rice at 14% *EMC*. By introducing the model into a computerized heat and mass transfer balance, it would be possible to refrigerate a silo of rice automatically under safe conditions with non-conditioned air. Zomordian (2001) predicted *EMC* of three Iranian rice cultivars (champa, domsiah and salari) using empirical models. The best results were derived when the Henderson model was used, because the highest value of R^2 and the lowest value of error were derived by this model.

The FFBP neural network was used to create a relation between input and output of patterns. For investigation of the effect of different threshold functions on network optimisation, two strategies including similar and various threshold functions for all layers were used (Table 3). Both strategies were used for FFBP network with LM learning algorithm. The best results of using network and algorithm for first and second strategies are shown in Table 3.

Three and four layers FFBP neural networks were used for the prediction of *EMC*. The best result for three layers network and first strategy with TANSIG threshold function was 2-4-1 topology. This topology produces MSE=0.0000287, R^2= 0.9895 and E_{mr} = 5.96%. The best for LOGSIG threshold function was for 2-5-1, that produces MSE=0.0000226, R^2=0.9903 and E_{mr}=5.50%. Thus, the application of LOGSIG for first strategy gives the best result for three-layer network. The best result for four-layer network and first strategy with TANSIG threshold function was for 2-4-4-1 which produces MSE=0.0000235, R^2=0.9886 and E_{mr}= 6.07%. In this case, for LOGSIG threshold function, 2-4-3-1 threshold function had MSE=0.0000180, R^2=0.993 and E_{mr}=4.08%.

In the case of the first strategy, four-layer network with 2-4-3-1 topology produced the best values of MSE, R^2 and E_{mr}. The second strategy, with threshold function order of TANSIG-TANSIG-PURELIN for four layers and 2-4-3-1 topology, produced MSE=0.0000153, R^2=0.9958 and E_{mr} = 3.56. Comparison of the first and second results showed that the second strategy was better than the first one. Figure 2 shows a good fit between the experimental and predicted data values for the second strategy result. Training and testing process of patterns proved that the distribution and selection of training and data sets was done in a suitable way, because the values of two data sets had little difference in all training processes (Fig. 3). Comparison between prediction and experimental values of testing data set shows the optimized ANN that produced a low real error (Fig. 4). These results also show that the overtraining phenomenon has not occurred.

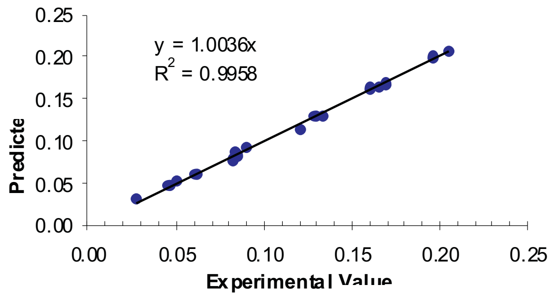

Fig. 2. Predicted values and real errors of optimized ANN for evaluation data.

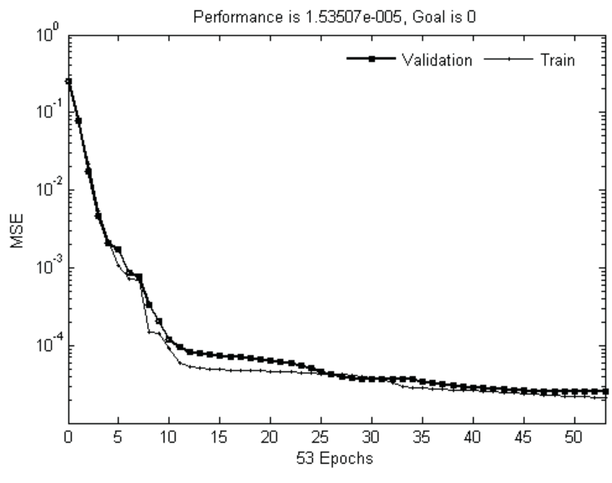

Fig. 3. Mean square error of training and testing patterns for the best ANN.

Comparison of the best result of mathematical model which is related to modified Chung-Pfost and the best result of ANN which is related to FFBP network, LM algorithm, 2-4-3-1 topology and second strategy with TANSIG-TANSIG-PURELIN showed that the ANN approach was more suitable, since its value of (0.9958) was higher than that of the Chung-Pfost model (0.9861) and its value of E_{mr} (3.56) was lower than the Chung-Pfost model (4.76) (Fig. 5). Chen and Jayas (1998) recommended that models producing E_{mr} lower than 5 are better to be considered as a good fit. Results of the ANNs and mathematical methods have this criterion, but the ANN method presented a unique model and the mathematical method presented eight models, so and is the average of those models.

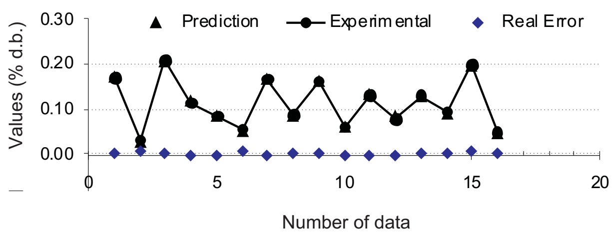

Fig. 4. Predicted values of *EMC* using ANNs versus experimental values and real error.

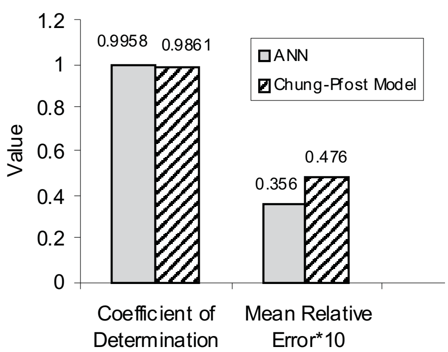

Fig. 5. Best results of R^2 and E_{mr} for the Chung-Pfost model and optimized ANN.

CONCLUSIONS

1. The results showed that the *EMC* of rough rice could be predicted by ANNs, with lower mean relative error and higher coefficient of determination compared to the mathematical models.

2. The best result for mathematical model belonged to the modified Chung-Pfost model, with R^2=0.9861 and E_{mr} =4.76.

3. The best ANNs for data training was FFBP with LM algorithm and TANSIG-TANSIG-PURELIN threshold functions for layers, four neurons for the first hidden layer and three neurons for the second hidden layer.

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