Development of ANN based sorption isotherm algorithm for the prediction of EMC of the paddy

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Abstract: A sorption isotherm algorithm based on artificial neural network (ANN) was developed for the prediction of equilibrium moisture content (EMC) of paddy under low temperature conditions (20°C to 40°C). ANN architecture was modeled by considering water activity (a_w) and temperature (T) as input and EMC as output neurons. A sorption isotherm experiment under low temperature conditions viz. 20°C, 25°C, 30°C and 35°C was conducted for providing training, testing and validation data of ANN. 2-7-1 was selected as the best ANN architecture on the basis of which sorption isotherm algorithm was developed in MATLAB R2015a. Mathematical modeling was also performed for the analysis of sorption isotherm behavior. Among four models as applied for the analysis, modified Chung-Pfost model showed best results with coefficient of determination (R^2) value of 0.98 and mean square error (MSE) value of 8.82×10^{-05}. Hence, this study involves a pioneering approach in the post harvest modeling aspect of sorption isotherm study of paddy.

Keywords: general algorithm, paddy, modified Chung-Pfost, ANN, sorption isotherm

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1 Introduction

Handling of rice is very difficult due its use for most of the human consumptions. It is due to the fact that market value of rice is affected by grain breakage and head rice yield. Mode of drying mainly affects the final product quality in terms of head rice yield. For preserving grain quality, various steps were adopted during the drying of paddy (Cnossen and Siebenmorgen, 2000; Cnossen et al., 2003).

For describing the complex processes involved during drying, mathematical model is an important tool. Knowledge of equilibrium moisture content (EMC) at different drying conditions is required for the simulation of drying process. During simulation, instead of using discrete EMC value at different drying conditions, predicted EMC values are derived from a previously known relationship between EMC vs. temperature and relative humidity in the form of sorption isotherm equation (Sun and Woods, 1994; Sun, 1999).

Sorption isotherm equations are used to predict the moisture sorption properties of food. In order to describe the sorption characteristics of food, many empirical and semi-empirical equations are proposed in literature. This is attributed due to the fact that different mechanisms in various water activity regions are involved for the water

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associated with the food matrix (Jayas and Mazza,1993). Mono-layer based kinetic models (BET model), multi-layer and condensed film kinetic models (GAB model), semi-empirical (Ferro-Fontan, Henderson and Hasley models) and empirical models (Smith and Oswin models) are mostly used for the sorption isotherm analysis of food material. For describing the interpretation of multilayer sorption isotherms particularly Types II and III, BET model represents a fundamental milestone (Sun, 1999). BET model is modified by many researchers for giving a good fit up to 0.9 water activity (Aguerre et al., 1989). GAB model is considered as the most versatile model for describing sorption isotherm behavior of food (Bizo, 1983; Timmermann, 1989). Sorption isotherm behaviors of 92 different food products are described by Ferro-Fontan equation (Iglesias and Chirife, 1995). It is attributed that a four term model can be used effectively for describing the sigmoid and non-sigmoid isotherms (Park et al., 1994). In order to describe the sorption isotherm behavior of biological materials such as starch and cellulose, Smith model can be used (San Martin et al., 2001). A semi-empirical model is proposed by Henderson for the equilibrium moisture content of cereal grains (Henderson, 1952). Hasley and Oswin models are also designated as versatile models (Chirife and Iglesias, 1978). Bennaceur et al. (2015) classified the various models of moisture sorption isotherms into the following broad categories: semi-empirical (Ferro-Fontan, Henderson, and Halsey), empirical (Smith and Oswin), and kinetic (Mod-BET, multilayer and condensed film), and monolayer (BET). The GAB model is widely used to describe the correlation between equilibrium moisture content (EMC) and water activity , and it has gained widespread acceptance across a variety of water activity values (Mahanti et al., 2019).

Although, all such models may be used for describing sorption isotherm behavior of different biological materials, but none of them can be claimed as the general sorption isotherm model for the cereal grains (Chen and Morey, 1989). Chirife and Iglesias (1978) evaluated eight models for 39 foods, where they reported proper predicted behavior of the models for specific crops under given ranges of temperature and relative humidity. Therefore it is necessary to select proper sorption isotherm model for a specific crop (Basunia and Abe, 2001; Chen and Jayas, 1998; Sopade and Ajisegiri, 1994).

In order to remedy this shortcoming, general class nonlinear models of ANN have been proposed (Mahanti et al., 2019). There is general agreement that these heuristic models are helpful for nonparametric regression and dynamic modelling. Estimation of parameters of these models is done by using nonlinear direct optimization techniques. Accuracy and shape of the isotherms as well as reliability of the predictions over the ranges of relative humidity are limited under such kind of estimations. So, an alternative computational method viz. artificial neural network (ANN) was used in order to predict sorption isotherm behavior of agricultural products. ANN model is based on a simplified model of human brain function. Without the availability of priori models, ANN can internally self-adapt and relate complex non-linear relationships between input and output variables. If a phenomenological model of the process is not available or too complex to derive, ANN modeling becomes more useful. In many food and agricultural applications such as psychometry (Smith, 1947), drying (Henderson, 1952), thermal processing (Peleg, 1993), rheology and sensory science (Park et al., 1994), ANN concepts were successfully applied. Besides that, ANN modeling is applicable for the interpretation of data recorded during normal productions. Hence, ANN can be preferred as an alternative for the modeling of such processes (Chakraborty et al., 2019; Chakraborty et al., 2020; Chakraborty et al., 2021; Gupta et al., 2021; Mahanti et al., 2019).

The objectives of this study were application of ANN for the sorption isotherm kinetics of paddy, comparison between the ANN and mathematical models and development of a general algorithm for the prediction of EMC of the paddy.

2 Materials and methods

2.1 Paddy sample

Medium variety of paddy viz.'Aijung' (*Oryza sativa Linn)* was used for the sorption isotherm analysis. The paddy samples were collected from the local market of Tezpur University, Assam, India (Longitude: 26.7003 °N, Altitude: 92.8308 °E.

2.2 Sorption isotherm analysis of paddy

Sorption isotherm analysis of the paddy was done by dynamic method. For the analysis water activity meter was used. Total nine paddy samples (moisture content ranging from 12% to 28%wb) were prepared. The samples were analyzed in the closed chamber of water activity meter at different temperatures viz. 20 ℃, 25 ℃, 30 ℃ and 35 ℃. At the end of each run, water activity of the sample was determined. The water activity meter (Make: Aqualab) had water activity and sample temperature range of 0.030-1.000 and 15 ℃-50 ℃ respectively.

2.3 Mathematical modeling of the sorption isotherm kinetics

Modeling of sorption isotherm of paddy was done by taking EMC as a function of water activity (a_w) and temperature (T). For the Modeling of grains and grain sorption equilibrium data modified Chung-Pfost, modified Hasley, modified Henderson and modified Oswin models were successfully used. GAB model was recommended for using in food laboratories in Europe (Van Den Berg, 1984) due to its versatility in predicting sorption isotherm behavior (Timmermann, 1989; Jayas and Mazza, 1993). Also in case of modeling of sorption isotherm of grains, GAB model showed successful performance (Jayas and Mazza, 1993; Ruan et al., 1995; Sun, 1999; San Martin et al., 2001). The original model was proposed without the temperature term (De Boer, 1953; Anderson, 1946; Cnossen et al., 2003). So a modified GAB model was developed with inclusion of temperature and six constant terms (Aviara et al., 2004; Iguaz and Virseda, 2007). Evaluation of the mathematical models was done on the basis of coefficient of determination (R^2) and mean square error (MSE) values. Table 1 shows the mathematical models used for the sorption isotherm analysis of paddy.

Table 1 Mathematical models used for the sorption isotherm analysis

Model Name	Equation	References
Modified Henderson	$M_e = \left[\frac{-\ln(1-a_w)}{A(T+B)}\right]^{\frac{1}{C}}$	(Henderson, 1952; Thompson et al., 1968)
Modified Chung and Pfost	$M_e = -\frac{1}{C} ln\left[\left(-\frac{T+B}{A}\right) ln(a_w)\right]$	(Chung and Pfost, 1967)
Modified Hasley	$M_e = \left[-\frac{\exp(A+BT)}{\ln(a_w)}\right]^{\frac{1}{C}}$	(Hasley, 1948; Chirife and Iglesias, 1978)
Modified GAB model	$M_e = \frac{AB\left(\frac{C}{T}\right)a_w}{(1-Ba_w)\left[1-Ba_w+\left(\frac{C}{T}\right)Ba_w\right]}$	(Anderson, 1946; De Boer, 1953;Zou et al., 2016;Jayas and Mazza, 1993)

Note: M_e=equilibrium moisture content (% d.b), a_w=water activity in decimal and A, B and C are equation coefficients

2.4 Modeling of sorption isotherm kinetics by using artificial neural network (ANN)

ANN model is developed based on the behavior of natural neuron. ANN architecture consists of five important components viz. input layer, hidden layer, summation function, threshold function and output layer. Processing of ANN is carried out with the help of different connecting weights.. In Neural network, W_{ih} are the inter connection weights of the input (L_I) and hidden (L_H) layers, whereas W_{ho} are the inter connection weights of the hidden (L_H) and output (L_O) layers. Best ANN architecture is selected by employing back propagation algorithm. Minimization of error is considered as the parameter for the selection of the architecture. In ANN architecture, the outputs of j^{th} neuron for hidden and output layers are denoted by H_{oj} and O_j respectively (Bhadra et al., 2010; Chakraborty et al., 2016). ANN architecture in connection with different processing elements is shown in Figure 1.

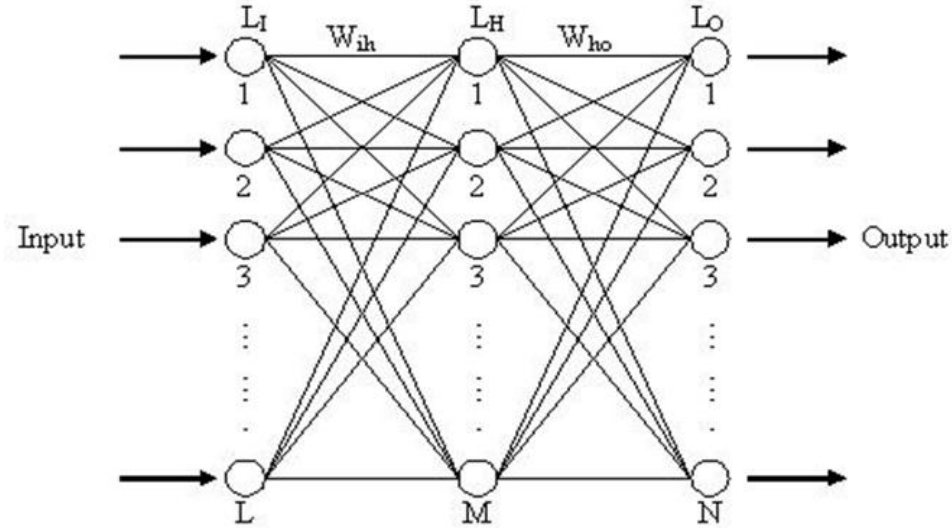


Figure 1 Schematic diagram of ANN general architecture

H_{ij} denotes total input for j^{th}neuron to hidden units. The equation for H_{ij} is shown in Equation 1

$$H_{ij} = \sum_i X_i W_{ij} \qquad (1)$$

Here, X stands for input of ANN and W refers to weight of the network connecting input and hidden layers

Real-value output of the hidden unit is denoted by H_{oj}. Bias (T_j) values are also introduced as extra inputs to hidden (T_h) and output (T_o) units. The output of the j^{th}neuron from the hidden to output layer is given by the following equation

$$H_{oj} = \frac{2}{1+e^{-2(H_{ij}+T_h)}} - 1 \qquad (2)$$

The final output of the output layer namely O_j is determined by using equation 3

$$O_j = W_{ho} H_{oj} + T_o \qquad (3)$$

In the present study, the experimental data were divided into three parts viz. training, testing and validation. Total 2000 iterations were used during each run with a learning rate varied from 0.5 to 1. ANN modeling was executed in MATLAB R2015a. The best ANN architecture was selected on the basis of mean square error (MSE) and coefficient of determination (R^2) values.

3 Results and discussions

3.1 Experimental sorption isotherm behavior of paddy

Type-II isotherm behavior was observed for the paddy under low temperature conditions (20 ℃, 25 ℃, 30 ℃ and 35 ℃). It could be also observed that water activity (a_w) of the paddy increased with the increase in temperature (T) at constant equilibrium moisture content (EMC). Besides at constant temperature (T), positive effect of EMC on a_w of the paddy can also be observed. Figure 2 demonstrates the sorption isotherm behavior of the paddy under low temperature conditions.

3.2 Mathematical modeling of the sorption isotherm kinetics

Statistical results of the mathematical models, used for the sorption isotherm kinetics of paddy are illustrated in tabulated form. Among all the models, Modified Chung and Pfost model showed the best performance with highest $\boldsymbol{R^2}$ value of 0.98 and lowest MSE value of 8.82×10^{-05}. Experimental data along with temperature effect were fitted in a better way by using modified Chung-Pfost model. Modified GAB model was unable to give better results due to the reason that monolayer constant value (A) is very high as compared to the literature explained by Chen and Jayas (1998). Table 2 represents the statistical results of the mathematical models.

3.3 Application of ANN for the modeling of sorption isotherm kinetics

For attaining generalized model with best adequacy, ANN modeling was also applied to model sorption isotherm behavior of paddy. Total 108 data were considered as input of ANN architecture. The experimental data were divided into three parts viz. 70% for training, 15% for testing and 15% for validation respectively. For each architecture, total 10 runs were carried out. Based on the average MSE value as obtained for each architecture, best ANN architecture (2-7-1) was selected. The selection of ANN architecture is illustrated in Figure 3. Figure 4 shows the best ANN architecture, 2-7-1. The plots between the experimental and ANN/NN (artificial neural network/neural network) predicted sorption isotherm behavior of paddy are shown in Figure 5 (a-d). The prediction behavior of ANN shows R^2 value of >0.99. Hence, this model can be applied to predict EMC of the paddy on the basis of water activity (a_w) and temperature (T).

From Figure 4, it can be also observed that sorption isotherm behavior of the paddy samples under all the conditions shows similar type of trend namely Type- II pattern. It can be also noticed that EMC decreases with the increase in temperature at constant water activity, and increases with the increase in water activity, at constant temperature.

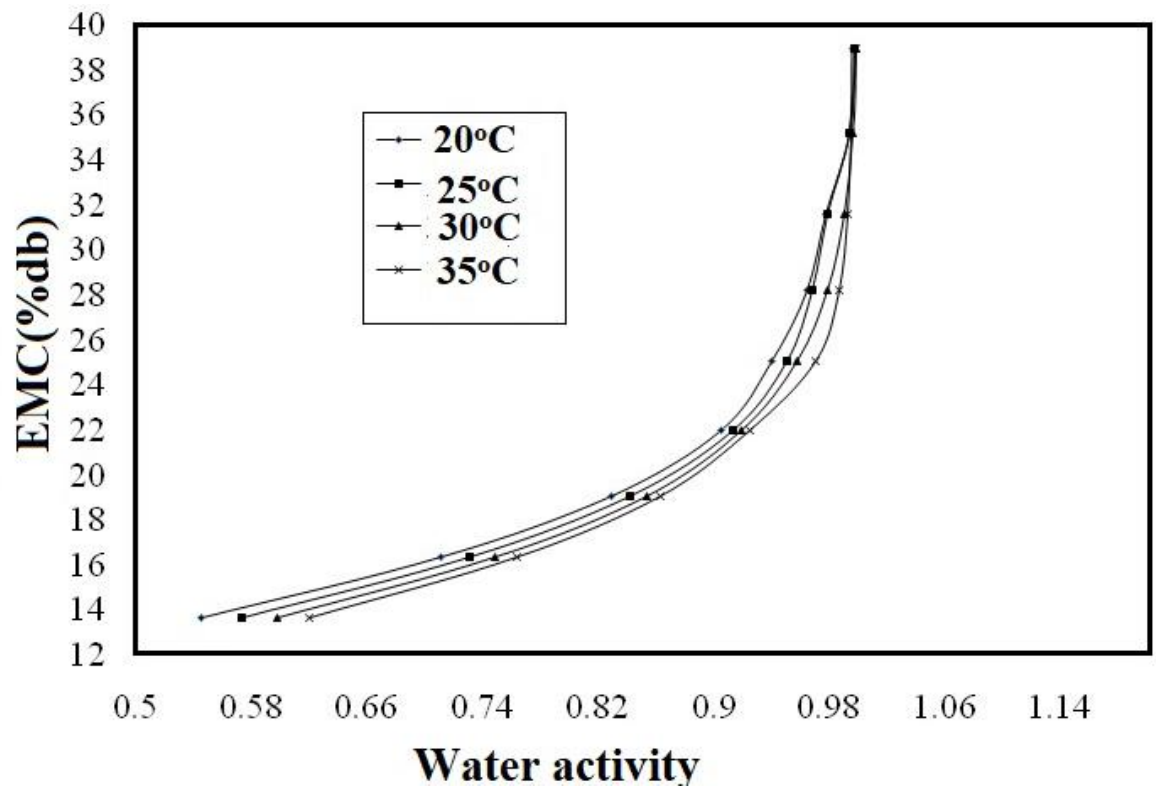


Figure 2 Sorption isotherms of paddy at different temperatures (20 ℃, 25 ℃, 30 ℃ and 35 ℃)

Table 2 Statistical results of the mathematical models fitted for the sorption isotherm analysis

Model name	Model constants			Statistical parameters	
	A	B	C	R^2	MSE
Modified Chung and Pfost	1.12	2.43	1.73	0.98	$8.82X10^{-05}$
Modified Henderson	$3.22X10^{-06}$	5263.19	1.60	0.97	$2.46X10^{-05}$
Modified Hasley	2.80	0.01	5.38	0.96	$2.88\ X10^{-05}$
Modified GAB	3815	0.88	0.05	0.97	0.02

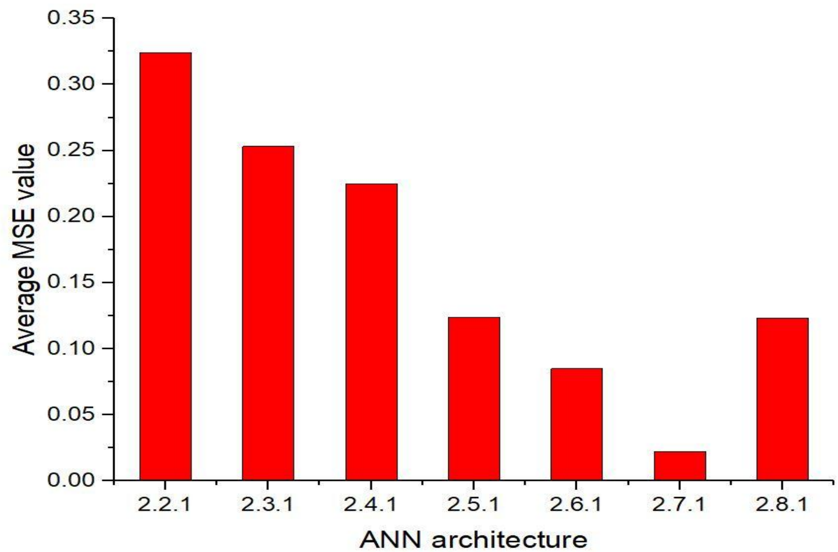


Figure 3 Selection of ANN architecture.

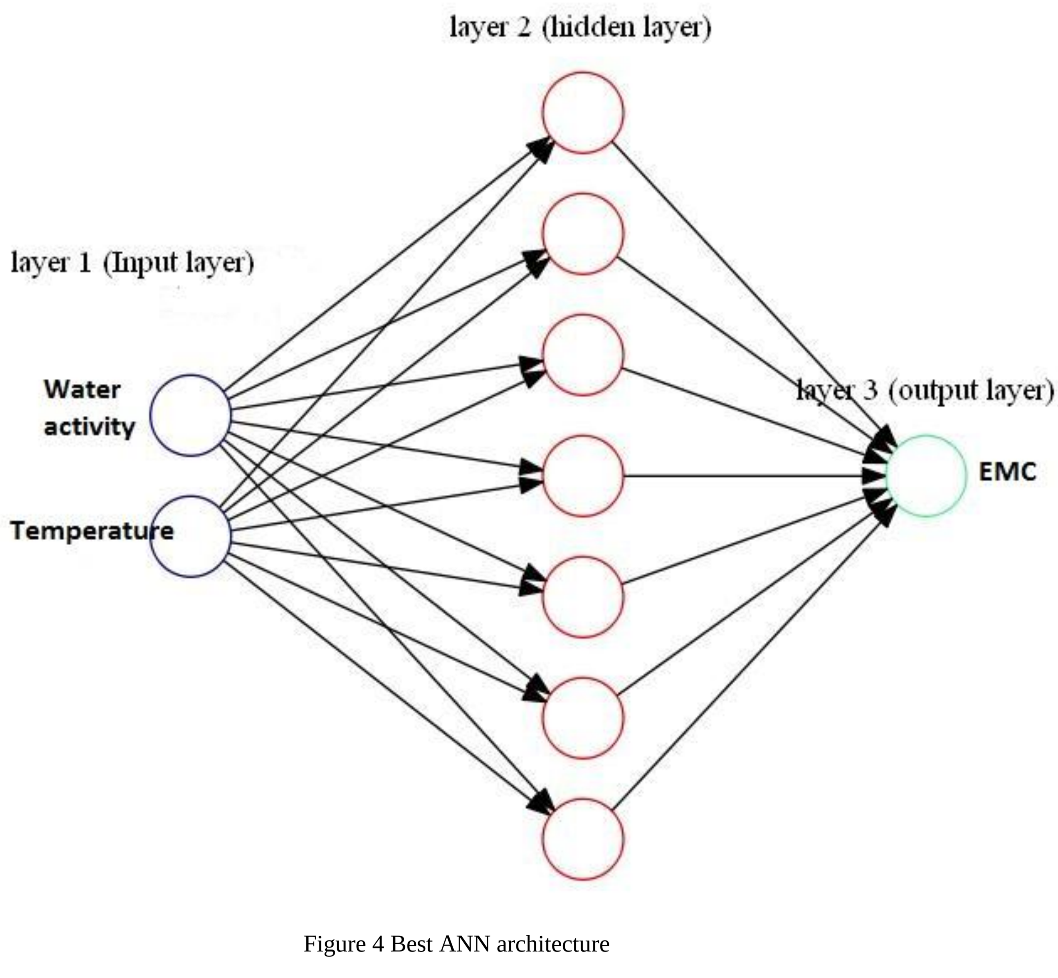
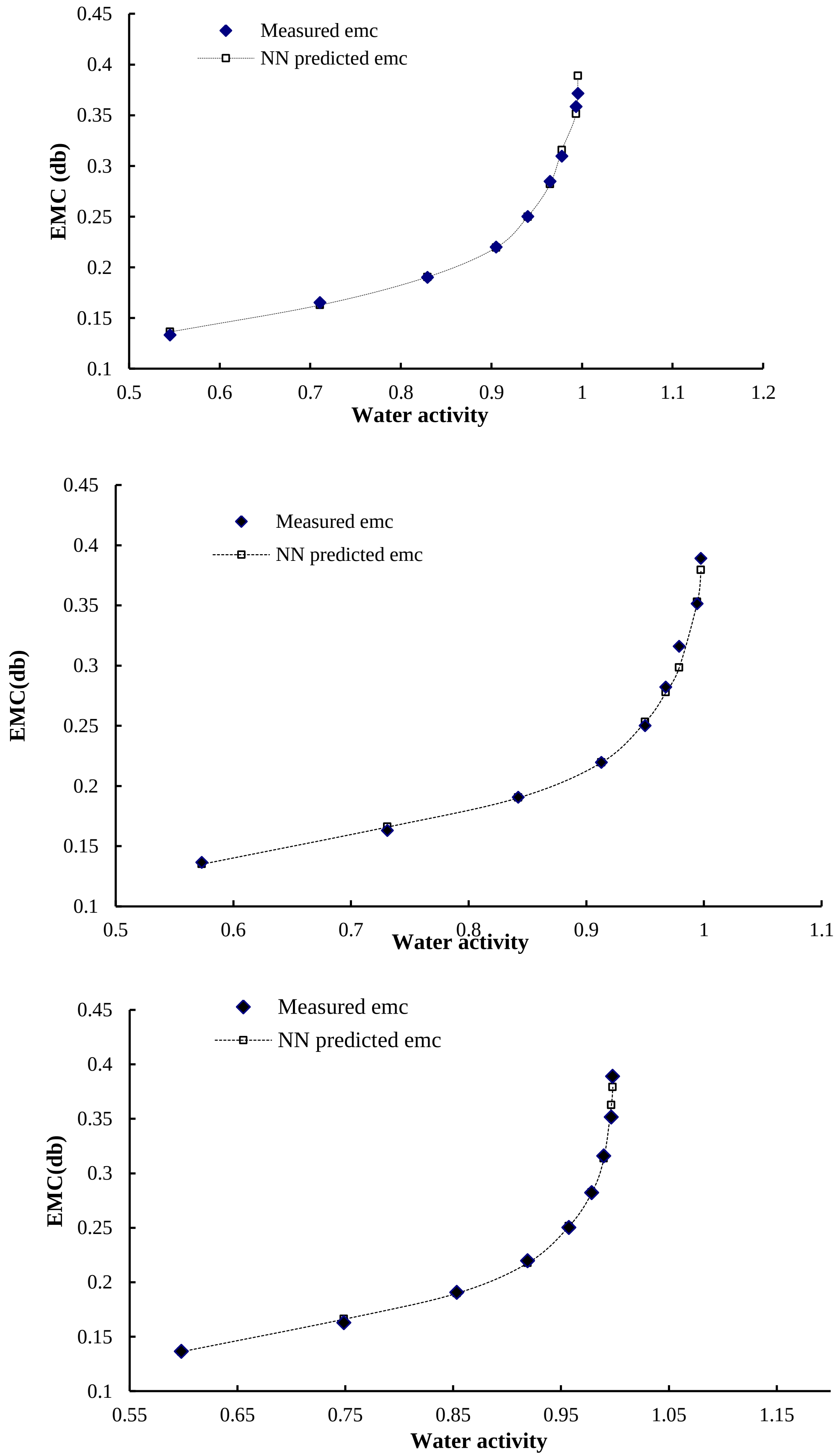


Figure 4 Best ANN architecture



Measured emc
NN predicted emc
EMC (db)
Water activity
Measured emc
NN predicted emc
EMC(db)
Water activity
Measured emc
NN predicted emc
EMC(db)
Water activity

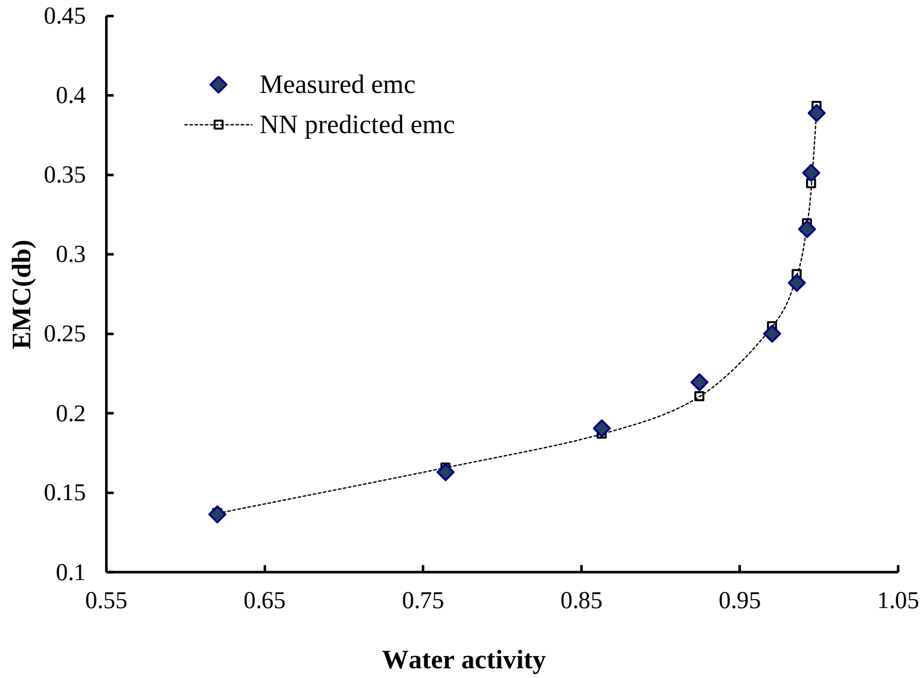


Figure 5 Plot between experimental and ANN/NN predicted sorption isotherm behavior of paddy at (a) 20°C (b) 25°C (c) 30°C (d) 35°C

3.4 ANN based sorption isotherm algorithm for the determination of EMC of the paddy

For predicting EMC of the paddy as a function of water activity (a_w) and temperature (T), a sorption isotherm algorithm was developed on the basis of weight and bias values of the best ANN architecture (2-7-1). This algorithm was programmed in MATLAB R2015a. In order to determine EMC of the paddy under low temperature conditions (20°C -35°C), this algorithm can be utilized as an effective tool. The MATLAB code of the sorption isotherm algorithm is given as follows:

```
function [EMC] = sorption_algorithm (input)
INP=input
p = reshape (INP,2,1);
maxp= reshape(maxp,2,1);
minp= reshape(minp,2,1);
INP = 2*(p-minp)./(maxp-minp) - 1;
INP=reshape (INP, 2,1);
WH = [13.4099782526318, 9.31429125314798; …
3.57896005964360,5.40591883529437; …
0.435039575766513,1.77923051634133;
0.739992665334911,-2.87576912278052;
0.711256333330143,6.39511058019858;
0.443272287815504,-4.66982595941145;
0.856855969290288,40.4487653485315];
WO = [-0.0169524103982516, 0.0394670447190306, …
0.261406995173906, -0.147053726338591, …
0.0737601046465460, -1.71251922276934, …
7.47632357222974];
BH = [0.0296147557692265;-5.95698328927511; …
-0.872188895839435;-1.15414622408570;
5.52459564276327;5.64035775131541;
-41.5763233283774];
BO = [8.72044018483660];
pnn = WO*tanh(WH*INP+BH)+BO;
EMC = 0.5 *(pnn+1)*(maxpo-minpo) + minpo;
%%maxp &minp are maximum and minimum input ranges
%%maxo &mono are maximum and minimum output ranges
%%% EMC is the normalized output
```

4 Conclusion

In this study, sorption isotherm behavior of the paddy was investigated under the low temperature conditions. Experimental results showed type-II isotherm behavior for all the conditions. From the results it can be revealed that water activity of the paddy increased with the increase in temperature at constant EMC, whereas with the increase of EMC, water activity increased at constant temperature. Four mathematical models were used for the modeling of sorption isotherm behavior. Among these models, modified Chung-Pfost showed best performance with highest R^2 value of 0.98 and lowest MSE value of 8.82×10^{-05}. In order to develop a relationship between EMC vs. water activity (a_w) and temperature (T), ANN modeling was applied. 2-7-1 was selected as the best ANN architecture. A general sorption algorithm on the basis of best ANN architecture was also developed for predicting EMC of the paddy under low temperature conditions.

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