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Mathematical models for moisture sorption isotherms of barley and wheat

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Abstract

Moisture sorption isotherms play an essential role in the preservation and storage of dehydrated foods. To study the behavior of different cereals (wheat, barley) in a certain equilibrium static environment gravimetric methods were applied for temperatures between 16 and 25°C and water activity varying from 0.533 to 0.909. The moisture isotherms were sigmoid shaped and showed a clear dependence of temperature with water activity (a_w). GAB and a second order polynomial equation were used to model the experimental data.

Keywords: sorption isotherms; equilibrium state, water activity, GAB, polynomial models

1. Introduction

Knowledge of the sorption characteristics is essential to: understand the stability in storage and acceptability of food products, drying process modeling, design and optimization of drying equipment, aeration, calculation of moisture changes which may occur during storage, and for selecting appropriate packaging materials [1-2] have reported the static gravimetric technique as the preferred method for determining the moisture sorption isotherms of food products.

This method has several advantages over the manometric and hygrometric techniques, and these are: ability to determine the exact dry weight of the sample, minimization of temperature fluctuation between samples and their surroundings or the source of water vapor, registering the weight change of the sample in equilibrium with the respective water vapor pressures, and achieving hygroscopic and thermal equilibrium between samples and water vapor source. The differences in experimental techniques adopted affect the sorption properties of foods [3]. Saturated salt solutions are commonly used to create the necessary micro-climate for the sorption experiments. This has necessitated the production of template-like data to prepare the standard solutions referred to by several researchers [4-5]. The main aim of this study was to determine the sorption isotherms of barley and wheat grains over a range of temperatures and humidity commonly experienced in the mild environment.

The specific objectives include the presentation of the influence of temperature on sorption isotherms, and modeling of the adsorption moisture isotherms using two widely recommended isotherm models.

2. Materials and Method

Material preparation. Wheat (Dropia) and barley (Andrei) from SCDA Company, BRAILA, was harvested in spring, 2008.

The wheat had an initial moisture content and aw of 8,72 ± 0.45 kg/100kg dry matter, and 0,578 ± 0.015, and the barley had an initial moisture content and aw of 6,74 ± 0.45 kg/100kg dry matter, and 0,533 ±

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0.015, respectively. The grains were kept in cold storage at 7°C until use. Initial moisture content (m.c.) of the grains was determined in duplicate according to the AOAC (1990) procedures.

Micro-climate. The required micro-climate was prepared based on previous experience by using six saturated salt solutions (NaCl, KCl, HN_4Cl, K_2SO_4, KNO_3, $(NH_4)_2SO_4$ and different relative humidity's were selected to give different a_w values in the wheat and barley. The relative humidity/a_w values of the salt solutions at different temperatures are those indicated in other researches [6].

Determination of adsorption isotherms. To determine adsorption isotherms the static gravimetric method was used. Three replicates of wheat and barley (15 and 10 g), sufficient to give a uniform single layer in the glass containers used as moisture pans, were placed in desiccators at each a_w point and temperature level. The desiccators were placed in a Binder Incubator to maintain the required temperature. Samples were monitored for equilibration by weighing at intervals, until constant weights were attained. The moisture content of the equilibrated samples (the e.m.c.) was then found by calculation from the initial m.c. and the known change in weight [7].

Isotherm equations and modeling. Two widely recommended isotherm equations (GAB and Polynomial) that were investigated with the experimental data are shown in Table 1 in the form M = f (a_w,T), where M is the moisture content. The SAS procedure for non-linear regression (Proc NLIN) was used.

Table 1. Models used to describe the sorption isotherms

Model	*Equation*
GAB	$M = \frac{m_0 C K a_w}{[(1 - K a_w)(1 - K a_w + C K a_w)]}$
Polinomial	$M = a + b a_w + c a_w^2$

a: constant, *k*: constant, a_w: water activity, *b*: constant, c: constant, *C*: GAB model parameter, *K*: GAB model parameter, m_0: monolayer moisture content (kg/100kg dry matter).

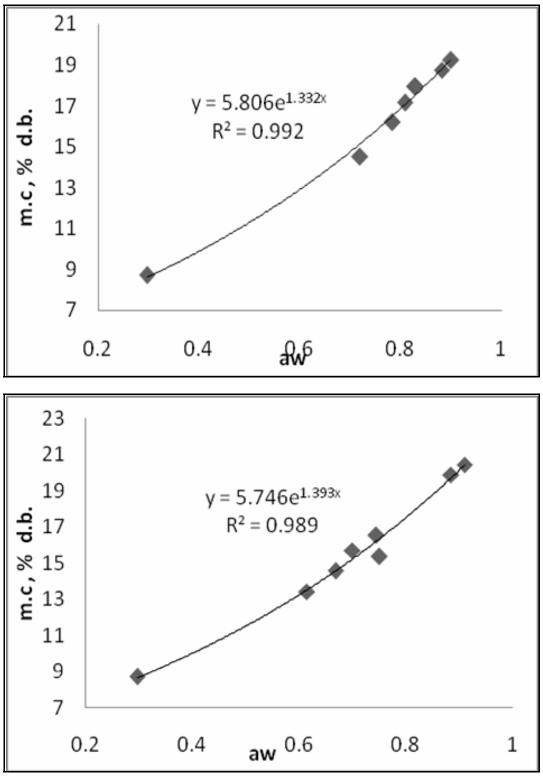
The goodness of fit of the models was evaluated by means of the mean relative percentage deviation modulus (P), defined as:

$$P(\%) = \frac{100}{N} \sum_{i=1}^{N} \frac{|M_{ei} - M_{ci}|}{M_{ei}} \quad (1)$$

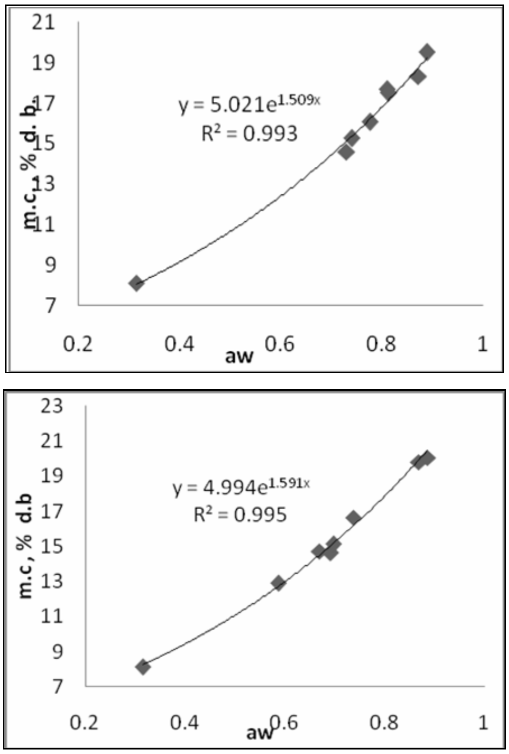
where M_{ei} and M_{ci} are the experimental and predicted moisture content values, respectively, and N is the number of experimental data. A model is considered acceptable if it has a P value less than 10% .

3. Results and Discussion

The adsorption and desorption isotherms at 16, 25°C are shown in Fig. 1. The isotherms have a sigmoid shape depicting an increase in the equilibrium moisture content with a_w. This are typical Type II isotherms [8] and has been reported for starchy products such as potato and wheat starch [7].



(a)



(b)

Figure 1. Adsorption isotherms a) wheat b)barley

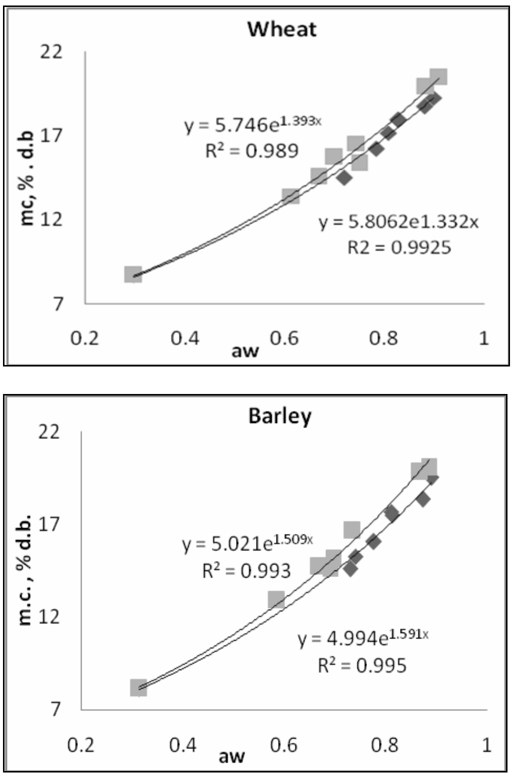


Figure 2. Adsorption isotherms for wheat and barley at 16 (◆) and 25ºC(■)

The correlation between aw and moisture content for wheat at 25ºC is significant (R2=0.989), while the correlation coefficients for wheat at 16 ºC and barley at 16 and 25 ºC is highly significant. (R2=0.99). An exponential equation was used to depict the relationship between moisture and aw.

The temperature dependence of the sorption isotherms can be seen in Fig. 2 where the equilibrium moisture content is observed to decrease with decrease in temperature, at the same aw, and aw is seen to decrease with temperature increase, at the same equilibrium moisture content. This indicates that the wheat and barley becomes less hygroscopic when temperature is increased.

For example, for wheat at 16.07% dry base the aw is of 0.777 at 16 ºC and of 0.722 at 25 ºC.

Tables 2 and 3 shows the coefficients of the models fitted to the experimental adsorption data by non-linear regression and P (%) the mean relative percentage deviation modulus. The correlation coefficients (R^2) were in all cases higher than 0.985.

Table 2. Mathematical models for the adsorption isotherms of wheat

Model	**Temperature(°C)**	
	16	25
GAB		
C	19,7036	13,8212
K	0,6433	0,6253
m_0	8,5221	9,3396
P(%)	1,70	1,78
R^2	0,999	0,999
Polinomial		
a	8,3420	6,9412
b	-4,3753	1,7329
c	18,6443	14,4240
P(%)	1,48	1,63
R^2	0,988	0,980

Both models has P <10% so they can be considered reliable to describe the correlation between a_w and moisture content at 16ºC and 25ºC. Moreover, the statistical parameters computed for the model and R^2 indicates a good estimation of the parameters for the experimental values.

The estimated monolayer moisture content (m_0) from the adsorption isotherms using GAB equation is of 8.5221 and 9.3395 kg/100 kg for wheat at 16 and 25 ºC, respectively and higher for barley, of 9.3395 and 10.4305 at 16 and 25 ºC. These values are in line with the values reported by Yanniotis (1994) for high starchy foods between 20 and 30ºC (7.36 kg/100kg).

The accuracy of the models and its concomitant parameters was evaluated plotting the experimental values versus the predicted ones for each studied temperature (16 and 25ºC).

From the figures 3 and 4 a good correlation between predicted and experimental values was observed.

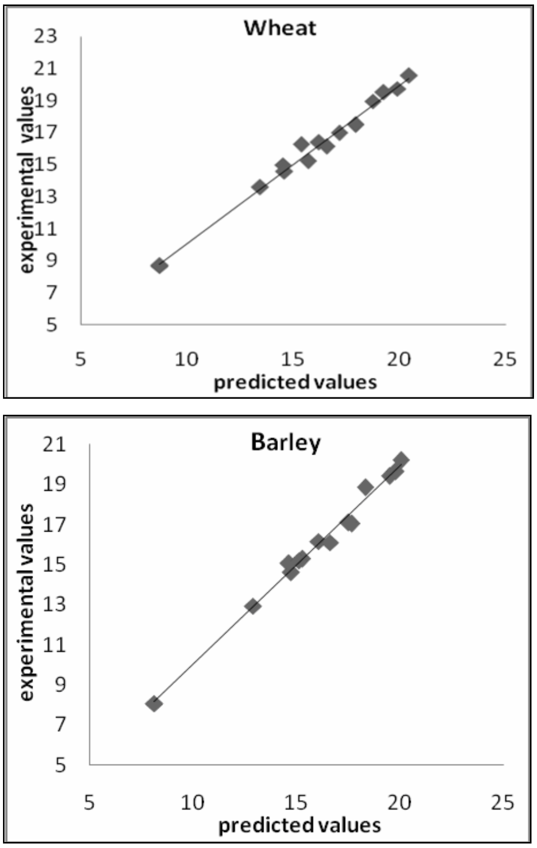


Figure 3. Relationship between the experimental and predicted relative humidity values for GAB model

Moreover, the deviation of bisector line can be considered an indicator for the model fitness. Since a concentration of the data can be noticed along with the bisector line we can conclude that all the models (GAB and Polynomial) accurately describe the experimental data behavior. Hence, it could be concluded that the proposed models and its parameters accurately described the adsorption isotherms for both wheat and barley.

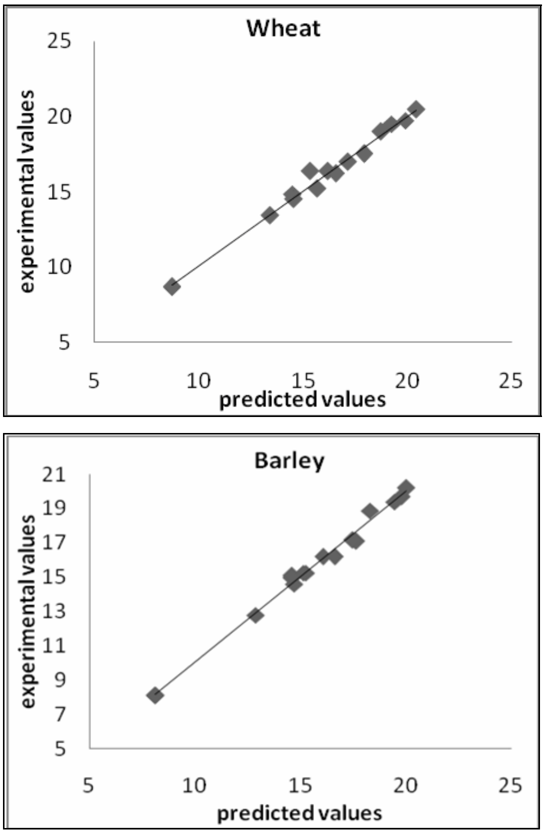


***Figure* 4.** Relationship between the experimental and predicted relative humidity values for the Polinomial model

Graphics of the residual values (differences between experimental and predicted values) shows no signs of bias as results from figures 5 and 6.

The random distribution of residuals for wheat and barley is an indicator that demonstrates the correspondence between theoretical and experimental values.

4. Conclusion

Adsorption isotherms for wheat and barley at 16 and 25 ºC have sigmoid shape and behave like Type II isotherms;

Temperature has a significant influence on sorption isotherms, and an increase in a_w values was noticed for the same humidity content with temperature decrease;

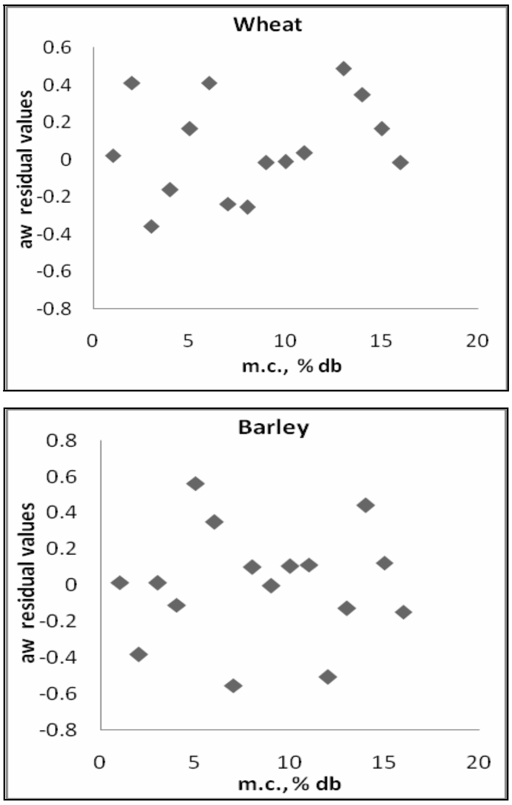


Figura 5. Residual a_w values for Polinomial model

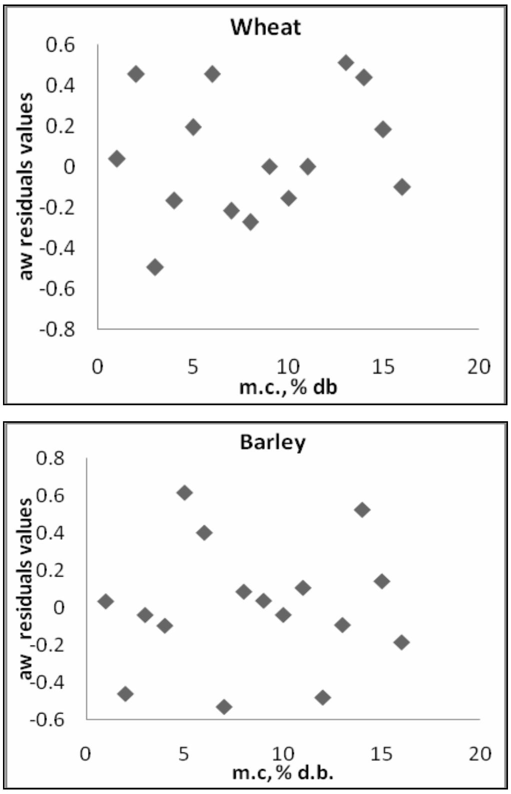


Figura6. Residual a_w values for GAB model

The experimental values could be modeled using GAB and Polinomial models using the non linear regression;

For all cereals, models and all experimental temperatures the convergence criteria was met;

The estimated parameters are in line with other similar researches for other cereals;

The relationship diagrams of the experimental and predicted values, the residual distribution charts and the correlation coefficients (R^2) and P(%) were appropriate and indicates good accuracy of the models used.

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