Experimental Determination and Modeling of Desorption Isotherms of the Tomato "Lycopersicum esculentum"

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Authors’ contributions:

This work was carried out in collaboration among all authors. Author RL designed the study, wrote the protocol, and wrote the first draft of the manuscript. Authors GGN and SO managed the analyses of the study. Authors KP, FO and SK managed the literature searches. All authors read and approved the final manuscript.

ABSTRACT

The aim of this work is to make a contribution to the drying of tomatoes. The purpose of this contribution is the experimental determination of the desorption isotherms of a variety of tomato (one of the most widespread on the Burkinabe market place) using the static gravimetric method at temperatures of 25°C, 40°C and 50°C. It is more specifically a question of validating a theoretical model based on these experimental studies. Sorption isotherms allow us to have information to establish the stability of food products and their storage conditions.
These isotherms are curves which give valuable information on the hygroscopic balance of a product because they allow to know its range of stability after drying by determining the final water content.

Keywords: Isotherms; desorption; drying; water content; experimental; modeling.

1. INTRODUCTION

Sorption isotherms represent the relationship between the water content of a food and the activity of water at a given temperature.

Furthermore, to optimize the storage conditions of a product so as to ensure its physico-chemical and microbiological stability, the determination of sorption isotherms is a necessity.

Several research studies [1,2,3,4] have described the determination of desorption isotherms for food products. However, very little work has been devoted to determining the isotherms of desorption of the tomato. The objective of this study is to determine the isothermal desorption isotherms of the *Lycopersicum esculentum* using the static gravimetric method at temperatures of 25°C, 40°C and 50°C. More specifically, it will be:

- determine the isotherms of desorption of the tomato;
- to model the desorption isotherms obtained.

2. MATERIALS AND METHODS

2.1 Sample Preparation

The tomatoes used in this study come from the fruit market in Ouagadougou, the capital of Burkina Faso. The Mongal variety is the one that was used in our study. To prepare the samples, good quality fruit (neither too ripe nor too raw) was chosen, washed and rinsed with potable water. The tomatoes were then cut into slices about 1 cm thick.

2.2 Methods

The determination of the desorption isotherms of the tomato was carried out by the static gravimetric method. This method ensures consistency of the relative humidity in the environment in which the product is located, for a given temperature.

The experiments were carried out at 03 (three) different temperatures: 25°C, 40°C and 50°C and with 05 (five) standard saturated saline solutions.

To carry out our experiment, we used in this work an oven MEMMERT UFP 600 filled with 05 glass desiccators, containing different saturated saline solutions which are classified by increasing order of relative humidity: KOH, MgCl₂, NaNO₃, NaCl, KCl according to French standard NFX15-119, [5]. Table 1 presents the standard values for water activity (this is the ratio between the water vapor pressure at the surface of the product and the saturated vapor pressure, therefore without unit) as a function of the 5 salts used and depending on the temperature for determining the sorption curves.

To obtain the points of the desorption isotherm, samples cut into rings (1 cm) are placed in aluminum cups previously weighed. The “sample-dish” pairs are then weighed before being placed in the desiccators stored in the oven maintained at constant temperature. At given time intervals, weighings are carried out every 30 min using an PCE-B1H 6000 electronic balance with 0.001 g scale precision, until the mass variation between two successive measurements is practically zero (less than 1%).

| Saline solutions | T=25°C | T=40°C | T=50°C |
|------------------|--------|--------|--------|
| KOH              | 0,082  | 0,063  | 0,057  |
| MgCl₂            | 0,328  | 0,316  | 0,305  |
| NaNO₃            | 0,74   | 0,710  | 0,6904 |
| NaCl             | 0,753  | 0,747  | 0,744  |
| KCl              | 0,843  | 0,823  | 0,812  |

*Note. Water activity is without unit*
Table 1. Mathematical models used

| Models       | Equations                                                                 | Parameters |
|--------------|---------------------------------------------------------------------------|------------|
| HENDERSÖN   | \[ X = \left( \frac{-\ln \left(1 - A_w\right)}{A} \right)^{\frac{1}{B}} \] | A, B       |
| GAB          | \[ X = \frac{X_mCKA_w}{\left(1 - K\right)A_w + CKA_w} \]                  | Xm, K, C   |
| BET          | \[ X = \frac{X_mCA_w}{\left(1 - A_w\right) + CA_w} \]                    | Xm, C      |
| OSWIN        | \[ X = A\left(\frac{A_w}{1 - A_w}\right)^{\frac{1}{B}} \]              | A, B       |
| PELEG        | \[ X = K_1A_w^{n_1} + K_2\left(\frac{A_w}{1 - A_w}\right)^{n_2} \]      | K1, K2, n1, n2 |

Once equilibrium has been reached, the samples are then placed in an MEMMERT UFP 600 oven at 70°C for 48 hours [6] to determine their dry masses (ms). The equilibrium water content of the product is determined by:

\[ \omega_{eq} = \frac{m_{eq} - m_s}{m_s} \]

\( m_{eq} \) is the equilibrium mass of the product; \( m_s \) is the dry mass of the product.

For each desiccator, we define a couple \((\omega_{eq}, A_w)\) representing a point on the desorption isotherm curve.

### 2.3 Isothermal Modeling and Statistical Selection Criteria

In order to interpret the sorption curves obtained, 08 (eight) models (Table 2) described in the literature were used for the adjustment of the desorption isotherms of the tomato **Lycopersicum esculentum**. The modeling of desorption isotherms requires statistical methods of regression and correlation analysis. The correlation coefficient \( R^2 \) and the RMSE mean square error allowed us to choose the best equation which best describes the isotherm of desorption of the tomato **Lycopersicum esculentum** [7].

- The correlation coefficient \( R^2 \):

\[ R^2 = 1 - \frac{\sum_{i=1}^{n}(X_{i,exp} - X_{i,pre})^2}{\sum_{i=1}^{n}(X_{i,pre} - \bar{X}_{i,pre})^2} \]

- The RMSE mean square error:

\[ RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n}(X_{i,pre} - X_{i,exp})^2} \]

The various adjustments to experimental data were made using the Levenberg-Marquardt optimization algorithm under MATLAB version R2016a.

### 3. RESULTS AND DISCUSSION

#### 3.1 Experimental Determination

Fig. 1 shows, in the same reference, the experimental results obtained for desorption isotherms of the **Lycopersicum esculentum** tomato at \( T = 25°C \), \( T = 40°C \) and \( T = 50°C \). The initial water content of the tomato was 94.6% or 18.37 kg water/kg of dry matter.

This figure represents the evolution of the equilibrium water content as a function of the water activity of the salts used and this, as a
function of the temperatures of 25°C, 40°C and 50°C.

It is observed that, in general, the equilibrium water content increases with the activity of the water.

So it can be said that water activity and temperature have a significant effect on the equilibrium water content. These results obtained are similar with other results reported in the literature [16,1].

Also, we observe that for the same water activity, the higher the temperature, the more the equilibrium water content decreases. This shows that the temperature has an influence on the isotherms of the tomato.

So we can say that the temperature has a significant effect on the equilibrium water content. The same result was found by Nasfi N. and al. [4] for the Laurel.

3.2 Modeling of Desorption Isotherms

Figs. 2, 3 and 4 show the adjustments of the desorption isotherms determined experimentally by the theoretical models GAB and PELEG described in Table 2 at T = 25°C, T = 40°C and T = 50°C.

![Graph showing desorption isotherms at different temperatures](image)

**Fig. 1. Isotherms of desorption of the tomato "Lycopersicum esculentum" at T=25°C, 40°C and 50°C**

**Fig. 2.a. Isothermal Desorption T=25°C:** Experimental points and simulated curves

**Fig. 2.b. Isothermal Desorption T=25°C:** Experimental points and simulated curves GAB model PELEG model
Figs. 2, 3 and 4 show a good correlation between the theoretical and experimental values with the various adjustments of experimental data that were made using the Levenberg-Marquardt optimization algorithm under MATLAB version R2016a.

The more the water activity increases, the water content assumes higher and higher values which gives an increasing polynomial appearance to the different curves according to the model considered. Whatever the model considered, the curves have the same appearance. The difference between these models lies in the values of the correlation coefficient $R^2$ and the RMSE mean square error. These said values are grouped in Table 3.

The best model will be the one with the highest $R^2$ value and the lowest RMSE value.
## Table 3. Values of the estimated parameters and selection criteria

| Models  | T  | 25°C | Parameters | R²  | RMSE  | 40°C | Parameters | R²  | RMSE  | 50°C | Parameters |
|---------|----|------|------------|-----|-------|------|------------|-----|-------|------|------------|
|          | R² | RMSE | a=2.577    | b=0.6909 | 0.9982 | 0.01165 | a=2.375    | b=0.5607 | 0.9985 | 0.009221 | a=2.39      |
| HENDERSON | 0.9966 | 0.01628 | b=0.6909 | 0.9982 | 0.01165 | a=2.375 | b=0.5607 | 0.9985 | 0.009221 | a=2.39      |
| GAB      | 0.9972 | 0.01808 | a=0.6113 | b=0.7899 | 0.9988 | 0.01135 | a=1.787 | b=0.8203 | 0.9990 | 0.009400 | a=0.6257    |
| BET      | 0.9900 | 0.02799 | a=0.1097 | b=2.507 | 0.9971 | 0.01456 | a=0.1235 | b=1.302 | 0.9985 | 0.009146 | a=0.1273    |
| OSWIN    | 0.9939 | 0.02183 | a=0.1618 | b=0.8145 | 0.9972 | 0.01438 | a=0.1272 | b=0.9827 | 0.9983 | 0.009653 | a=0.1034    |
| PELEG    | 0.9990 | 0.01562 | a=1.085 | b=0.06779 | n1=3.956 | 0.9925 | 0.04036 | a=5.984 | b=4.83 | n1=3.194 | 0.9995 | 0.009079 | a=0.4275    |
| HASLEY   | 0.9868 | 0.03224 | a=0.1105 | b=1.004 | 0.9931 | 0.02233 | a=1.231 | b=0.8469 | 0.9957 | 0.01564 | a=0.1233    |
| LANGMIR  | 0.9873 | 0.03877 | a=1006 | b=1006 | c=125.5 | 0.9888 | 0.03496 | a=1310 | b=1310 | c=121.7 | 0.9819 | 0.03912 | a=501.8      |
| IGLESIAS | 0.9868 | 0.03229 | a=0.02627 | b=0.1181 | 0.9971 | 0.01452 | a=0.001653 | b=0.1238 | 0.9974 | 0.01215 | a=-0.006721 |
By comparing the correlation coefficient $R^2$ and the RMSE mean square error obtained for each model, we could conclude, from Table 3, that the Peleg model is the most suitable model for fitting the desorption isotherms of the tomato "Lycopersicum esculentum" with values of $R^2 = 0.9995$ and RMSE = 0.009079 for relative humidities between 5.7% and 81.2%.

For relative humidities between 6.3% and 82.3%, the GAB model also describes these desorption isotherms for the tomato "Lycopersicum esculentum" with values of $R^2 = 0.9988$ and RMSE = 0.01135. Studies by Anderson [17] and Caceres [18] have shown that among the theoretical approaches, the Brunauer, Emmet and Teller (BET) equation best describes the isotherm of products with low water content and that of its extension, called the GAB model, allows the sorption isotherm of highly porous food products, like tomatoes, to be completely adjusted over the entire range of water content.

4. CONCLUSION

The present study was carried out with the aim of determining the desorption isotherms of the Mongal tomato variety by the gravimetric method for three temperatures (25°C, 40°C and 50°C).

Fitting of the experimental results by different models found in the literature using the MATLAB software, it was found that the Peleg model is in our study the most adequate model to describe the isotherm of desorption of the tomato "Lycopersicum esculentum" and therefore to explain the hygroscopic behavior during the conservation of this variety of tomatoes. Within the framework of his study on the determination of desorption isotherms, Ahouannou, C. and al in [19] affirm that Oswin's theoretical model makes it possible to reproduce as well as possible the okra desorption isotherm. E. Ayranci, in [20], affirms on the other hand, that the GAB model, for its part, gives a better approach to its experimental results.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Jamali A, and al. Moisture adsorption-desorption isotherms of Citrus reticulata leaves at three temperatures. Journal of Food Engineering. 2006;77:71-78.
2. Ahouannou C, Jannot Y, Sanya E, Degan G. Experimental determination and modeling of desorption isotherms of tropical agricultural products. Africa Science. 2010;6(3):1-17.
3. Tiendrebeogo E. Study of the thermo-hydro-mechanical processes of isothermal drying of the micro-alga spirulina platensis "arthrospira platensis": Experience and modeling. Unique doctoral thesis, Joseph Ki-ZERBO University, Burkina faso. 2016:163.
4. Nasfi N, Bagane M. Détermination expérimentale et modélisation des isothermes de sorption du Laurus Nobilis. L du Sud Tunisien, Journal of Environmental Science, Toxicology and Food Technology. 2017;11(3)Ver. I:52-56.
5. Tiendrebeogo E. Study of the thermo-hydro-mechanical processes of isothermal drying of the micro-alga spirulina platensis "arthrospira platensis": Experience and modeling. Unique doctoral thesis, Joseph Ki-ZERBO University, Burkina faso. 2016:163.
6. AOAC. Official method of analysis 15th Edition. Journal of the Association of official Analytical Chemists. AOAC International: N° 934.06, Washington, DC. 1990;673.
7. Ertekin C, Yaldiz O. Drying of eggplant and selection of a suitable thin layer drying model. Journal of Food Engineering. 2004;63:349-359.
8. Henderson SM. A basic concept of equilibrium moisture. Agricultural Engineering. 1952;33:29–32.
9. Van den Berg C, Bruin S. Water activity and its estimation in food systems: Theoretical aspects. In L. B. Rockland & G.F. Stewart, Water activity: Influences on food quality. New York: Academic Press. 1981;1-43.
10. Brunauer S, Emmet PH, Teller E. Adsorption of gases in multimolecular layers. Journal of the American Chemical Society. 1938;60:309–319.
11. Oswin CR. The kinetics of package life. III. Isotherm. Journal of Society of Chemical Industry. 1946;65:419-421.
12. Peleg. Assessment of semi-empirical four parameter general model for sigmoid sorption isotherms. Journal of Food Processing Engineering. 1993;16(1):21-37.
13. Halsey G. Physical adsorption on non-uniform surfaces. Journal of Chemical Physics. 1948;16:931–937.
14. Langmuir I. Journal of American Chemical Society. 1916;46:1361-1362.
15. Iglesias HA, Chirife J. A model for describing the water sorption behavior of foods. Journal of Food Science. 1976;41:984–992.
16. Menkov ND, et al. Applying the linear equation of correlation of Brunauer Emmet-Teller (BET)-monolayer moisture content with temperature, Nahrung. 1999;43:118-121.
17. Anderson RB. Modifications of the brunauer, emmet and teller equations. American Chemical Society. 1946;68:686-691.
18. Caceres G. Modeling of the drying of a deformable saturated porous medium: Taking into account the liquid pressure. Doctoral thesis, University of Bordeaux. 2006;1:142
19. Ahouannou C, Jannot Y, Lips B, Lallemand A. Characterization and modeling of the drying of three tropical products: Cassava, Ginger and Okra Food Science. 2000; 20:413-432.
20. Ayranci E. Equilibrium moisture characteristics of dried eggplant and okra. Die Nahrung. 1995;39(3):228-233.