Physica A 400 (2014) 57–70

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

Modeling of adsorption isotherms of water vapor on Tunisian olive leaves using statistical mechanical formulation

S. Knani [a,*], F. Aouaini [a], N. Bahloul [b], M. Khalfaoui [a], M.A. Hachicha [a], A. Ben Lamine [a,1], N. Kechaou [b]

[a] Unité de Recherche de Physique Quantique, Faculté des Sciences de Monastir, Université de Monastir, Tunisie

[b] Groupe de Recherche en Génie des Procédés Agroalimentaires, Laboratoire de Recherche en Mécanique des Fluides Appliquée - Génie des Procédés - Environnement, Ecole Nationale d'Ingénieurs de Sfax, Université de Sfax, BP 1173, 3038, Sfax, Tunisie

HIGHLIGHTS

- New model was established to fit water isotherm in food products.
- The model is able to predict the topography of the water adsorbed molecules.
- Monolayer adsorbed quantity gives the capacity of olive leaves to retain water.
- The adsorption energy reflects the exothermic character of the adsorption of water.

ARTICLE INFO

Article history:
Received 24 March 2013
Received in revised form 18 November 2013
Available online 11 January 2014

Keywords:
Modeling
Statistical physics
Adsorption isotherm
Water activity
Olive leaves
Thermodynamic functions

ABSTRACT

Analytical expression for modeling water adsorption isotherms of food or agricultural products is developed using the statistical mechanics formalism. The model developed in this paper is further used to fit and interpret the isotherms of four varieties of Tunisian olive leaves called "Chemlali, Chemchali, Chetoui and Zarrazi". The parameters involved in the model such as the number of adsorbed water molecules per site, n, the receptor sites density, N_M, and the energetic parameters, a_1 and a_2, were determined by fitting the experimental adsorption isotherms at temperatures ranging from 303 to 323 K. We interpret the results of fitting. After that, the model is further applied to calculate thermodynamic functions which govern the adsorption mechanism such as entropy, the free enthalpy of Gibbs and the internal energy.

1. Introduction

The shelf life and safety of perishable products were related to the water content and especially to water activity (a_w) that determine the microbial safety and the physical texture of processed foods. The water activity (a_w) is defined as the ratio of partial pressure (p) of water vapor in air pressure and water vapor saturation (p_{vs}) in the same temperature. This informs on the availability of water molecules to participate in physical, chemical, and microbiological reactions [1–6].

* Corresponding author. Tel.: +216 97227351.
E-mail address: knanisalah@yahoo.fr (S. Knani).

[1] Present address: Department of Physics, Faculty of Sciences of Monastir, Boulevard de l'Environnement,5019 Monastir, Tunisie. Tel.: +21673500276; fax: +21673500278.

0378-4371/$ – see front matter © 2014 Elsevier B.V. All rights reserved.
http://dx.doi.org/10.1016/j.physa.2014.01.006

Nomenclature

Q	The equilibrium water content (kg water/kg dry matter).
Q_0	The monolayer water content on the internal surface (kg water/kg dry matter).
a_w	The water activity.
C	BET constant.
k	GAB constant.
Z_{gc}	The grand canonical partition function.
N_0	The average site occupation number.
ε_i	The receptor site adsorption energy.
μ	The chemical potential.
N_i	The receptor site occupation state.
k_B	The Boltzmann constant.
T	The absolute temperature.
N_M	The receptor sites per mass unit.
n	The number of molecules per site.
a_1 and a_2	Two dimensionless parameters which are related to the adsorption energy.
ΔE_1^a, ΔE_2^a	The molar adsorption energies at first and other layers respectively.
ΔE^v	The vaporization energy of one adsorbed mole of water molecules.
R^2	The coefficient of determination.
n_m	The number of moles of adsorbate in a monolayer.
a	The cross-sectional area of the water molecule (10.6×10^{23} m^2).
A_s	The surface area (m^2/kg solid).
M	The molecular mass of water (18 kg/kg mol).
N_A	Avogadro's number (6.02×10^{23} molecules/mol).
J	The grand potential.
S_a	The configurational entropy.
E_a	The total adsorption energy.
E_{int}	The internal energy.
G	The enthalpy of Gibbs.

The water content versus water activity data is important to predict the physical, chemical and biological changes that take place during the storage and processing of foodstuffs. At a fixed temperature, the water activity and corresponding water content are characterized by the water sorption isotherm. It can be obtained by one of two ways; adsorption or desorption. The two processes called sorption are not fully reversible, therefore a distinction can be made between the isotherms by determining whether the moisture levels within the product are increasing or decreasing [1,2,7,8]. The isotherms contain information about the sorption mechanism and the interaction of food biopolymers with water [6–12].

The modeling is very useful for describing and predicting sorption isotherms at various experimental conditions and therefore also useful for calculating thermodynamic properties that could be deduced. Then, experimental and theoretical studies of the water associated with agricultural products have been intensified in an attempt to understand and interpret water behavior.

We are interested in this work to the olive plant which has been an important source of nutrition and medicine in Tunisia. Olive leaves are known for their therapeutic and medicinal properties. They are used in both traditional and modern medicine. Indeed, they have been used as a medicinal herb to treat diabetic hyperglycemia, hypertension and infectious diseases [13]. It has also been reported that some components in these leaves are useful in preventing oxidative stress [14], radical-scavenging [15] and protecting low density lipoprotein from oxidation [16].

Olive leaves are a rich natural source of polyphenolic compounds which have biological activities such as antioxidant, antibacterial and antifungal properties [17]. Oleuropein is generally the most prominent phenolic compound in olive leaves and may reach concentrations of up to 60–90 mg/g of dry matter [18]. Oleuropein has antimicrobial activity against bacteria and parasites [19–21].

The quality of the leaves can be thereby seriously degraded within a few days. In fact, these changes are particularly influenced by moisture content of the material, relative humidity of ambient air and all biological materials over a wide range of relative humidity and temperature. Therefore, there is a need to select the most appropriate moisture sorption isotherm equation for a specific product and ranges of relative humidity and temperatures [18].

We focus this work on using the statistical physics approach to establish an expression of model giving the adsorbed water quantity versus the water activity. We apply the statistical model to fit experimental data of water adsorption isotherms onto Tunisian olive leaves at three temperatures 303, 313 and 323 K. We use also the results of fitting to interpret the adsorption process for each adsorption isotherm type, and then we relate the constants to the physicochemical parameters.