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Simplified algorithm for the prediction of water sorption isotherms of fruits, vegetables and legumes based upon chemical composition

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ABSTRACT

A simplified algorithm of prediction of water sorption isotherms for some foods was developed. This model is based on the composition of the main compounds of foods (glucose, fructose, sucrose, salt, protein, fibre and starch) and the influence of temperature was included (it was tested at 25 and 40 °C). Reported experimental data were employed as reference to validate the developed prediction model. Sorption isotherms for apple, apricot, banana, chestnut, loquat, quince, raisin, carrot, garlic, pepper, pumpkin, turnip, potato, bean, chickpea and lupine were predicted and compared to those reported in literature. The proposed model was able to predict the presence or absence of crossing between sorption isotherms at different temperatures for the same food. Using the prediction model could be calculated equilibrium moisture content with a determination coefficient (R^2) of (>0.982), a mean relative error (E) of (<9.43%) and a standard error (E_{RMS}) of (<0.042 kg (kg d.b.)$^{-1}$).

1. Introduction

From the point of view of its composition, a food can be defined as a multicomponent system constituted by a continuous aqueous phase and a small portion of scattered solids phases. The aqueous phase is dissolution of sugars, salts and other soluble compounds of low molecular weight. The scattered phase is constituted by non-soluble biopolymers such as starch, proteins, cellulose and other solid particles of complex composition (Martínez et al., 1998). Foodstuffs are strongly complex mixtures where each sample is unique (Spiess and Wolf, 1983). In order to establish a physical modelling of the system, it's necessary to assume some simplifications as, for example, the number of main components that must be included in the model. The total water content and its interaction with the rest of the components is a decisive factor for modelling the systems by a simplified model. This is always the first step to be able to describe physical phenomena, such as mass transfer processes and the evolution of the system within a specified period of the food processing, drying or storage.

Thermodynamic state of water in foods is represented by the water activity as a function of moisture content at constant temperature and pressure. This relationship is known as water sorption isotherms. Moisture content and water activity data are important to predict the physical, chemical and biological changes that take place during the storage and processing of foodstuffs. In the literature is possible to find a large number of experimental studies of sorption isotherms. It would be expected that with all food sorption isotherms available in the literature, researcher could have enough equilibrium data of any food. However, this is not completely correct. The values of equilibrium moisture content given by different experimental sorption isotherms reported in the literature show a great discrepancy (Herman et al., 1999; Roman et al., 2004). In this way, it would be of great importance to achieve isotherms obtained through theoretical considerations (Crapiste and Rotstein, 1982).

Spiess and Wolf (1983) and Myhara et al. (1998a) determined that the chemical composition plays an important role in the behaviour of the water sorption of food, and particularly in the case of vegetables. Sugar solution can bind water, such that the water is less able to contribute to the partial pressure of water vapour. Consequently, as these sugar solutions increase in concentration, the resulting water activity will be decreased. As the temperature of this sugar solutions increases, the water activity for a given equilibrium moisture content, will also increase (Goula et al., 2008).

Experimental isotherms reported in the literature are based on the determination of three physical properties: equilibrium moisture content, water activity and temperature (commonly at atmospheric pressure). There are empirical and semi-empirical equations to establish mathematical relationships among these three variables (Iglesias and Chirife, 1978), which are usually evaluated by the adjustment of the experimental data. Other possibility is the prediction of water activity, at each moisture content and temperature, from some fundamental laws and empirical expressions (Gal, 1975).

Water activity of a solution or a food that behaves like a solution, in terms of the characteristics of the solute (electrolyte or non-electrolyte) can be calculated very accurately, known moisture content of food and the concentration of the main solutes.

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Nomenclature

A	Henderson parameter (Eq. 16), (kg d.b.) kg^{-1}
A_Φ	Debye–Hückel parameter (Eq. 8)
a_w	Water activity
B	Henderson parameter (Eq. 16)
$B_\pm$	Characteristic parameter of each electrolyte (Eqs. 5 and 6)
b	Parameter of Eq. (8)
$C_\pm$	Characteristic parameter of each electrolyte (Eq. 5)
E	Mean relative percentage deviation modulus (%)
E_{RMS}	Root mean square error, kg (kg d.b.)$^{-1}$
F	Electrostatic parameter (Eqs. 5 and 8)
I	Ionic force, g mol^{-1}
K'	Norrish's constant (Eqs. 2 and 3)
M	Molecular weight, g mol^{-1}
m	molal
N	Number of samples (Eqs. 17 and 18)
R^2	Coefficient of determination
S	Solubility, g (100 $g_{solvent}$)$^{-1}$
T	Temperature, °C or K
X	Equilibrium moisture content (dry basis), kg (kg d.b.)$^{-1}$
X'	Equilibrium moisture content (wet basis), kg (kg w.b.)$^{-1}$
x	Molar fraction, mol (total mol)$^{-1}$
Z	Charge of the ions
z	Parameter of Eq. (11)

Subscripts

cal	Calculated
exp	Experimental
i	Number of the component
in	Non-soluble compounds
n	Number of components
o	Pre-exponential
rec	Recalculated
s	Solute
so	Soluble compounds
sup	Assumed
+, −	Charge of the ions
w	Water

Superscript

o	Reference state

Greek letters

α	Parameter of the Pitzer equation (Eq. 6)
β	Modified Henderson parameter (Eq. 9)
χ	Mass fraction, kg (kg total)$^{-1}$
Φ	Osmotic coefficient (Eqs. 4 and 5)
v	Number of ions in solution

Herman et al. (1999) reported an algorithm to predict pineapple sorption isotherms using the Ross equation by introducing the following considerations. Water activity produced by a single solute remains constant when this solute reaches the saturation concentration in the aqueous phase. The saturation concentration of a single solute is equal to its saturation concentration in a binary mixture with water. Water activity is calculated as a function of moisture content, chemical composition of product and temperature, that is, $a_w = f(X, \chi, T)$.

The main aims of this study are the development of a simplified algorithm that is able to predict the water sorption isotherms of foodstuffs at different temperatures by means of its chemical composition (mainly proteins, fibre, salt and carbohydrates (glucose, fructose, sucrose and starch)) and also validate the predictions by means of the corresponding comparisons with the sorption isotherms obtained from experimental data.

2. Materials and methods

The development of a prediction model involves three basic steps: the study of theoretical basis of model, the creation of the prediction algorithm and finally the validation and evaluation of prediction model that leads to the selection of an optimal configuration. In the third step the generation of the experimental data is necessary (or the compilation of available data in the literature) to fit the model.

2.1. Basic considerations to the development of the prediction model

In order to develop mathematically the proposed model, it's necessary to obtain a relationship between water activity and moisture content, taking into account food composition. The proposed algorithm includes some basic considerations. The calculation of water activities and moisture contents of soluble components (glucose, fructose, sucrose and potassium chloride) and non-soluble components (fibre, protein and starch) is different. The calculation is also different for electrolytes (potassium chloride) and non-electrolytes (glucose, fructose and sucrose) into soluble compounds.

A fundamental concept is the law of Raoult for ideal solutions, which shows that the water activity (a_w) is equal to water molar fraction (x_w):

$$a_w = x_w \tag{1}$$

An extension of the Raoult law for non-ideal solutions was developed by Norrish (1966) to calculate the water activity in binary solutions of sugars:

$$a_w = x_w \exp(K' x_s^2) \tag{2}$$

where x_s is the solute molar fraction and the empirical parameter K' is characteristic of a particular solute. The K' values for single solutes, typical in foods were already provided by Sloan and Labuza (1976). It is necessary to extend Norrish equation to multicomponent systems (Ross, 1975):

$$\ln(a_w) = \ln(x_w) - \left[(K'_i)^{1/2} x_{si} + \cdots\cdots\cdots + (K'_n)^{1/2} x_{sn}\right]^2 \tag{3}$$

Eq. (3), deduced by assuming negligible interactions between solutes, was applied by some authors (Chirife et al., 1985; Vega-Mercado et al., 1994; Myhara and Sablani, 2001) to predict the water activity of sugar mixtures, organic acids and foods with soluble and non-soluble solids with acceptable results. Lewicki (2000) developed on the basis of Raoult law a model of sorption isotherms. A recent trend, in development, for the prediction of food sorption isotherms, is the use of artificial neuronal networks. Myhara and Sablani (2001) developed a model sorption isotherms of several fruits (strawberries, grapes, figs, etc.), that involves up to 500 parameters of adjustment.

Water activity of the electrolytic solutions can be calculated by the following equation:

$$a_w = \exp(-0.018\, m v \phi) \tag{4}$$

where m is the molality, v is the number ionic species in solution and ϕ is the osmotic coefficient of the electrolytes compounds.