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A rapid and novel approach for predicting water sorption isotherms and isosteric heats of different meat types

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ABSTRACT

A rapid and novel approach for predicting sorption isotherms based on the Polanyi theory is proposed. This approach allows the prediction of the sorption isotherms at different temperatures from one experimental isotherm. The theoretical predictions of isotherms and isosteric heats were validated successfully using data from the literature for different meat types. This method allows total experimental time and operation costs to be reduced.

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1. Introduction

The influence of water on food reactions and food quality is important because the majority of biological reactions take place in aqueous media. Water content alone does not allow the evolution of many meat phenomena to be predicted; and the state of the water molecules in the food matrix is a better indicator (Clemente, Bon, Benendito, & Mulet, 2009).

Water activity in meat products is equivalent to the relative humidity of the air in equilibrium with the product. Knowing the state of the sorption-thermodynamic equilibria between the relative humidity of the surrounding air and the moisture content of the solid matter is a basic prerequisite for understanding mass transfer processes (Comaposada, Gou, & Arnau, 2000). Therefore, sorption isotherms and isosteric heats of sorption are important parameters in the design and modeling of sorption and drying processes, food engineering and industrial quality control, just as it is for any mass transfer situation (Delgado & Sun, 2001). Their correct determination represents a challenge to find an effective method to evaluate those parameters due to the intense development of processes.

The most widely used experimental method of obtaining the sorption equilibrium data of meat is a static method using a gravimeter (Comaposada et al., 2000; Wolf, Spiess, & Jung, 1985). In this method, the meat sample is exposed to atmospheres of known relative humidity that are controlled with different salts as proposed by Chirife and Resnik

* Corresponding author. E-mail address: farid.cortes@correo.upb.edu.co (F.B. Cortés). (1984) and Wolf et al. (1985) until there is no discernible weight change, indicating that the samples have reached equilibrium. The time required to acquire one experimental point, that is, the time required for the sample to equilibrate with the atmosphere, varied from 2 to 8 weeks based on the change in weight expressed on a dry basis (Chirife & Resnik, 1984; Clemente et al., 2009; Comaposada et al., 2000; Delgado & Sun, 2001; Delgado & Sun, 2002a, b; Kaymak-Ertekin & Gedik, 2004; Labuza, 2002; Singh, Rao, Anjaneyulu, & Patil, 2006; Wolf et al., 1985). Several experimental points are needed to construct one isotherm, requiring high acquisition times (Labuza, 2002). Complete knowledge of sorption isotherms is essential, and isotherms require experimental determination because current theoretical techniques are not able to accurately simulate systems as complex as foods (Kaymak-Ertekin & Saltanoglu, 2001).

Another important parameter is the isosteric heat of sorption, which is useful in assessing the energy needed for the drying process. Two methods can be used to determine the isosteric heat of sorption (Clemente et al., 2009): an indirect technique based on the sorption equilibrium data and estimation using calorimetric techniques and the Riedel equation (Riedel, 1977). The first method uses sorption experimental data (isotherms at different temperatures) to construct the sorption isosteres using a Clapeyron diagram and the Clausius-Clapeyron equation (Cortés, Chejne, Carrasco-Marín, Pérez-Cadenas, & Moreno-Castilla, 2010). The second technique requires accurate experimental work and expensive equipment. Therefore, the indirect method based on the Clausius-Clapeyron equation is the most widely used (Clemente et al., 2009; Comaposada et al., 2000; Cortés et al., 2010; Delgado & Sun, 2001; Delgado & Sun, 2002a, b; Kaymak-Ertekin & Gedik, 2004; Mulet, García-Reverter, Sanjuán, & Bon, 1999; Mulet, García-Pascual, Sanjuán, & García-Reverter, 2002; Singh et al., 2006).

Thus, in this work, a rapid novel approach for predicting experimental meat sorption isotherms based on the Polanyi theory (Polanyi, 1914, 1916) is proposed. The isosteric heats of sorption using the Clausius-Clapeyron equation from the estimated equilibrium data were computed. The main objective was to predict sorption properties of moisture sorption isotherms for different meat types at different temperatures from one isotherm, considerably reducing experimental time and operation costs.

2. Theoretical background

In 1914 a theory of adsorption was proposed to describe adsorption phenomena. This description is associated with Polanyi (Polanyi, 1914, 1916). The assumptions underlying the so-called potential theory of adsorption, commonly called the Polanyi theory, originate from earlier work by de Saussure, taken from Dabrowski (2001). According to this theory, the adsorbed layer is considered to be a thick multilayer film of decreasing density as the distance from the solid surface increases. The basic concepts of the Polanyi theory (Polanyi, 1914, 1916) include the adsorption potential and the characteristic adsorption curve. This characteristic curve presents a simple relationship between the adsorption potential and the distance from the solid surface (Fig. 1). This relationship is the characteristic adsorption equation (Eq. (1)). The aforementioned distance may be expressed in terms of volume units of the adsorbed phase. Polanyi (1914, 1916) assumed that the adsorption potential is also independent of temperature, meaning that the characteristic curve of adsorption of non-polar molecules is also temperature independent. Such a statement follows from the fact that the van der Waals forces are independent of temperature. The principal assumption of the theory is given by

$$\left(\frac{\partial A}{\partial T}\right)_{Y} = 0 \tag{1}$$

where T is temperature, X is moisture content and A is the adsorption potential.

Eq. (1) expresses the temperature invariance of the adsorption of different pairs as a function of the adsorption potential, a direct consequence of the Polanyi theory (Polanyi, 1914, 1916).

The adsorption potential is given by:

$$A = \overline{R}T \ln \left(\frac{P_{\rm s}}{P}\right) = -\overline{R}T \ln(a_{\rm w}) \tag{2}$$

where a_w is the steam activity considered as an ideal gas, R is the universal gas constant, P_s is the saturation pressure at a given temperature and P is the equilibrium pressure of water.

Having calculated the characteristic curve for a given temperature, it is possible to determine sorption isotherms at other temperatures. However, the Polanyi theory (Polanyi, 1914, 1916) does not give a definite equation for sorption isotherms that, to some extent, replace the characteristic sorption equation (Dabrowski, 2001; Dubinin, 1967).

The proposed method is based on the Polanyi theory (Polanyi, 1914, 1916). Taking Eq. (2) under isosteric conditions (X = constant), the sorption isosteres using only one experimental set of data can be constructed. Each equilibrium point i has the same value as the differential molar work of sorption,

$$\ln P_i = \ln P_{\rm si} - \left(\frac{T_1}{T_i}\right) \ln \left(\frac{P_{\rm s1}}{P_1}\right) \tag{3}$$

The expression in Eq. (3) allows construction of sorption isosteres (PT model), considerably reducing the time needed for any experimental method.

The isosteric heat *Q* can be obtained using the Clausius–Clapeyron equation (Cortés et al., 2010):

$$Q = \left(\frac{v_{\rm n}}{v_{\rm g}} - 1\right) \overline{R} Z \left(\frac{\partial \ln P}{\partial (1/T)}\right)_X \tag{4}$$

where P and T denote gas-phase equilibrium pressure of the sorbing species and the absolute temperature, respectively. Z is the compressibility coefficient (Z=1 for an ideal gas and Z \neq 1 for a real gas) and v_n and v_g denote the partial molar volume of the sorbing species in the sorption phase. For an ideal gas, Eq. (4) is simplified to (Cortés et al., 2010)

$$\left(\frac{\partial \ln P}{\partial (1/T)}\right)_{X} = -Q/R \tag{5}$$

The sorption equilibrium is comprehensively and fully described by isosteres, or (T, X, a_w) data sets, that are available over the entire sorbate concentration region. With this experimental data, it is possible to evaluate the isosteric heat of sorption using Eq. (5).

The accuracy of the fit was evaluated by calculating the root mean square percent error (*RMS*%).

$$RMS\% = 100*\sqrt{\frac{1}{n} \left[\sum_{1}^{n} \left(\frac{a_{\text{w-exp}} - a_{\text{w-cal}}}{a_{\text{w-exp}}} \right)^{2} \right]}$$
 (6)

where a_{w-exp} and a_{w-cal} are experimental and computed activity, respectively, and n is the observation number.

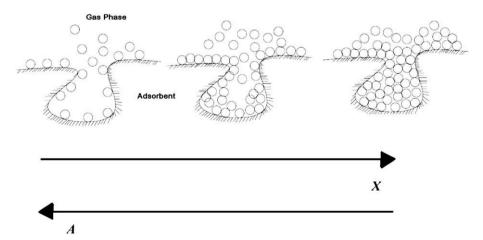


Fig. 1. Schematic of an adsorption system where the shaded molecules are the "captured" molecules under the influence of the van der Waals forces near to the pore surfaces.

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