Isotherms: software to simulate water sorption in foods

Abstract

Background: Food isotherms are considered important when evaluating in natura and industrialized products, as well as many processes associated with them. Although many water sorption models are available in the scientific literature for different food and agricultural products, freely accessible software is not available to estimate different isotherms in a custom developed application. This article describes a novel software tool, called Isotherms, capable of simulate the hygrosopic behavior of several foods based on an easy database management. The original database was mounted according to scientific studies previously published. The software was written in C++ programming language with an output including a table and a chart of the simulated isotherm. Results obtained for all the isotherms simulated by the software were compared against manual calculations performed in an electronic worksheet and available literature sources, demonstrating accurate results. Isotherms software also allows easy database updating and output saving due to the file formats which were considered during its implementation. The proposed computational tool is valuable to help students, engineers, researchers, and other professionals who work with food water activity and its relationship with industrial processes.

Keywords: mathematical models, water activity, food quality, adsorption, desorption

Introduction

The water sorption isotherm for a product is a graph where the moisture content is plotted as a function of water activity at constant temperature. Demarchi et al., Sorption describes both adsorption and desorption processes. Adsorption differs from desorption, since in the first process the product gains water while in the second one the product loses water. Sorption behavior of foods is considered as an important processing and storage parameter, since the stability of food products is directly related to their water activity. Generally, water activities below 0.6 protect food from degradation reactions, as well as, inhibit microorganism growth. The relationship between water activity and food moisture content is complex, depending on the food chemical composition. For this, numerous studies on sorption isotherms can be found in the literature for in natura and industrialized products. Among other biological software, desorption isotherms were obtained for green soybean, pear seeds, fresh beef, as well as anchovy in natura and enzymatic modified paste. Adsorption isotherms were determined for borojó fruits, orange juice powder, soluble coffee, and other several products. This relationship has been found to be useful in several applications, for example, for establishing the appropriate level of monolayer moisture content required for designing of drying process and storage conditions for black peppercorns. Another study dealt with the moisture sorption characteristics of tea stored in a chamber regulated by an atomizing humidification system. Also, the influence of sugar composition on sorption isotherms and on glass transition in apricots was evaluated. Despite the variety of water sorption models available and the numerous investigations on sorption isotherms that can be found in the scientific literature, freely accessible software is not available to estimate different sorption isotherms, considering different products, in a custom developed application. This article describes a novel software tool, called Isotherms. It is based on an extensive literature review and capable of simulate the hygrosopic behavior of several in natura and industrialized foods based on an easy database management.

Methods

The main sorption models were revised, as well as scientific studies to determine the experimental equilibrium moisture content of different food products at different temperatures and relative humidities. This information was compiled and a database was built containing on product identification, isotherm type (desorption or sorption), model identification, model equation, product temperature, model coefficients, and literature reference from which data were obtained. The main components of the Isotherms design are presented in Figure 1. The software was written in C++ language and is meant to read the database information, estimating the sorption curve of a registered product according to a pre-selected model and temperature. Simulation results can be visualized and exported. The data format of input (database) files supported is CSV (Comma Separated Values). According to Lardy et al., this file format is simple and widely used, also supported by almost all spreadsheet software and database management systems. Further, when using this file format, database updating and output analyses are facilitated. Output (result table and isotherm) is saved as electronic worksheet.

Several subroutines were built based on the Canvas class to draw the isotherms. The Canvas is pixel based and represents an image where graphics primitives such as rectangles, lines or polygons can be drawn onto. Thus, isotherm plots are directly drawn inside the application, according to the simulations performed by user. The application also controls when to draw the isotherm and what area needs to be redrawn when new simulations are made. Reading of the database and saving of results are done by using Variant data type, aiming at working with electronic worksheet and csv contents.
in a more flexible way. Additionally, during the database building phase, models identified with the same name and their coefficients were algebraically rearranged to a standard form in which results are expressed on decimal dry basis. This was required since many theoretical, semi-theoretical and empirical models to describe the sorption behavior of different food products have been proposed and applied in the literature. Thus, several researchers introduced or removed parameters in some of these models, as well as proposed changes in the structure of some equations, aiming at reaching a better fitting of the data, also expressing the water contents on percent dry basis or decimal dry basis. Results obtained for all the isotherms registered in proposed software database (Table 1) (Table 2) & (Table 3) were compared against manual calculations performed in an electronic worksheet and the available literature sources. This procedure totalized 209 tests.

**Figure 1** Structural design of the Isotherms software.

**Table 1** Products registered in the original database of Isotherms for desorption and adsorption curves

| Product      | Models                          | Reference       |
|--------------|---------------------------------|-----------------|
| Apple        | Halsey, Linear BET, Modified    | Kaymak-Ertekin  |
|              | Henderson, Oswin                |                 |
| Apricot      | Halsey, Linear BET, Modified    | Kaymak-Ertekin  |
|              | Henderson, Oswin                |                 |
| Bean         | Chung-Pfost, Copace, Modified   | Resende et al.  |
|              | Halsey, Modified Henderson,     |                 |
|              | Modified Oswin, Sigma-Copace    |                 |
| Chickpea     | Modified Chung-Pfost, Modified  | Menkov         |
|              | Halsey, Modified Henderson,     |                 |
|              | Modified Oswin                  |                 |
| Pink shrimp  | BET, GAB, Modified Smith,       |                |
| (dried)      | Hawrylak, Oswin                 |                 |
| Grape        | Halsey, Linear BET, Modified    | Kaymak-Ertekin  |
|              | Henderson, Oswin                |                 |
| Potato       | Halsey, Linear BET, Modified    | Kaymak-Ertekin  |
|              | Henderson, Oswin                |                 |
| Cactus pear  | BET, GAB, Henderson             | Campos et al.   |
| (protein     |                                 |                 |

**Table 2** Products registered in the original database of Isotherms for desorption curves

| Product      | Models                          | Reference       |
|--------------|---------------------------------|-----------------|
| Banana (pulp)| GAB                             | Staudt et al.   |
| Cauliflower  | GAB                             | Staudt et al.   |
| Mushroom     | GAB, Halsey, Henderson, Linear  | Kurozawa et al.|
| (fresh)      | BET, Modified Henderson,        |                 |
|              | Oswin                           |                 |
| Sapodilla    | GAB, Henderson, Linear BET      | Oliveira et al. |
| (lyophilized)|                                |                 |
| M. esculenta | GAB                             | Staudt et al.   |
| mushrooms    | GAB, Modified Henderson,        | Hubinger et al. |
| Atlantic bonito| fillet GAB, Modified Oswin,     |                 |
| (osmotically dehydrated) |                         |                 |
| Mushroom     | GAB, Linear BET, Halsey,        | Kurozawa et al.|
|              | Henderson, Modified Henderson,  |                 |
|              | Oswin                           |                 |
| Pistachio    | GAB                             | Staudt et al.   |
| nuts shell   |                                 |                 |
| Pupunha      | GAB                             | Ferreira et al. |
| (flour)      |                                 |                 |
| Rough rice   | GAB                             | Staudt et al.   |
| Tomato (pulp)| GAB                             | Staudt et al.   |

**Table 3** Products registered in the original database of Isotherms for adsorption curves

| Product      | Models                          | Reference       |
|--------------|---------------------------------|-----------------|
| Apricot (dried)| GAB                             | Staudt et al.   |
| Green beans  | GAB                             | Staudt et al.   |
| (dried)      |                                 |                 |
| Onion (dried)| GAB                             | Staudt et al.   |
| Cashew apple | BET, GAB, Henderson,            | Alcântara et al.|
| (dried)      | Modified Smith, Oswin           |                 |
| Red cherry   | GAB, Peleg                       | Vieira et al.   |
| (powder)     |                                 |                 |
| Coffee       | GAB, Chung-Pfost, Sigma-Copace  | Corrêa et al.   |
| (soluble)    | Smith                            |                 |

**Results**

The main screen of Isotherms is showed in Figure 2, allowing that user selects all the required data for the estimations. An output of the Isotherms software is illustrated by Figure 3, where user can view the isotherm table and curve. Additionally, in this module it is possible saving the data. Table 4 shows conversions used during the database building phase, when equations found in the scientific literature expressed the water content on percent dry basis. Table 5 presents the sorption models registered in the Isotherms. No universal sorption model is claimed for analyzing food and agricultural products, but the software database contains those often used for this purpose.
Figure 2 Main screen of the Isotherms software.

Figure 3 Output screen of the Isotherms software.

Table 4 Coefficient conversions used in the Isotherms software to express water content on dry basis

| Model           | D             | E             | F             |
|-----------------|---------------|---------------|---------------|
| BET             | D = A/100     | E = B         | F = C         |
| Chung-Pfost     | D = A/100     | E = B/100     | F = C         |
| Copace          | D = A - ln(100) | E = B         | F = C         |
| GAB             | D = A/100     | E = B         | F = C         |
| Halsey          | D = A        | E = B         | F = C         |
| Henderson       | D = A x 100 x B | E = B         | F = C         |
| Linear BET      | D = A/100     | E = B         | F = C         |
| Modified Chung-Pfost | D = A          | E = B         | F = C         |
| Modified Halsey | D = A - ln(100) x C | E = B      | F = C         |
| Modified Henderson | D = A x 100 x C | E = B       | F = C         |
| Modified Oswin  | D = A/100     | E = B/100     | F = C         |
| Modified Smith  | D = A/100     | E = B/100     | F = C         |
| Oswin           | D = A/100     | E = B         | F = C         |
| Peleg           | D = A/100     | E = B         | F = C/100     |
| Sabbah          | D = A/100     | E = B         | F = C         |

*D, E and F are the converted coefficients from an original equation in which the water content is expressed on percent dry basis. A, B and C are the coefficients of the original equation.

Table 5 Sorption models registered in the software database

| Model              | Equation                                                                 |
|--------------------|--------------------------------------------------------------------------|
| BET                | $U = \frac{(D \times F \times a_w (1 - a_w) \times X (1 - (F+1) \times a_w + F \times a_w^{F+1})}{(1 - (E \times a_w - E \times a_w^{E+1})}$ |
| Chung-Pfost        | $U = D \times E \times \ln(-T \times F \times a_w)$                      |
| Copace             | $U = \exp(D \times E \times T + F \times a_w)$                          |
| GAB                | $U = \frac{D \times E \times F \times a_w}{((1 - a_w) \times (-1 + (F \times a_w + E \times a_w)))}$ |
| Halsey             | $U = \left(-D \times \ln(a_w)\right)^{\frac{1}{E}}$                   |
| Henderson          | $U = \left(\frac{\ln(1 - a_w)}{D}\right)^{\frac{1}{E}}$                |
| Linear BET         | $U = \frac{D \times E \times a_w}{((1 - a_w) \times (1 + (E - 1) \times a_w))}$ |
| Modified Chung-Pfost | $U = \left(-\frac{1}{F}\right) \times \ln\left(\frac{T + E}{D \times \ln(a_w)}\right)$ |
| Modified Halsey    | $U = \left(\frac{\exp(D \times E \times T)}{\ln(a_w)}\right)^{\frac{1}{E}}$ |
| Modified Henderson | $U = \left(\frac{\ln(1 - a_w)}{D \times (T + E)}\right)^{\frac{1}{F}}$ |
| Modified Oswin     | $U = D \times E \times F \times \left(\frac{a_w}{1 - a_w}\right)^{\frac{1}{F}}$ |
| Modified Smith     | $U = D \times E \times a_w \times \log\left(1 - a_w\right)$              |
| Oswin              | $U = D \times a_w^{F} \times E \times a_w^{G}$                           |
| Peleg              | $U = D \times a_w^{E} \times F \times a_w^{G}$                           |
| Sabbah             | $U = D \times a_w^{E} \times F \times \exp(a_w)$                        |
| Sigma-Copace       | $U = \exp(D \times E \times T + F \times \exp(a_w))$                    |
| Smith              | $U = D \times E \times T - F \times \ln(1 - a_w)$                       |
Discussion

Isotherms software provides a friendly graphical user interface that can significantly reduce the user’s efforts for estimating and analyzing the food sorption curves from different models and/or for different products. When selecting data in the main screen of the software a database filter is applied, allowing a gradual and correct data selection. That is, when performing a new simulation set, user will select the product at first, and only them the sorption type (adsorption or desorption) will be enabled to be selected. After choosing the isotherm type, the models available for those product and isotherm type will be filtered and available to the user. Finally, after selecting the three first input data, it will be possible to inform or select the product temperature. In the case of a model that incorporate this parameter in the equation user can digit any temperature value, otherwise the temperatures available for the selected scenario will be available. All isotherms simulated by the proposed software present the water content on decimal dry basis. This unit is most commonly used for describing moisture variations in food, since when a sample loses or gains moisture this change is linearly related to the ratio of the weight of water to the weight of the dry matter. For this, water content is also given in gram per gram, which is equivalent to the decimal dry basis. When analyzing the isotherm results, the water content on percent dry basis can be divided by 100 and expressed on decimal dry basis. However, when using an equation which is originally calibrated for expressing results in percent dry basis, the coefficients need to be updated if the results must be expressed on decimal dry basis.

Regarding the registered models, according to Kaymak-Ertekin et al.,18 the BET, linear BET, and GAB models are considered the most used equations to describe water sorption in food materials. These models include the monolayer capacity (D coefficient in Isotherms) which constitutes an important parameter, directly related to the shelf life and stability of foods with regard to lipid oxidation, enzyme activity, non-enzymatic browning and structural characteristics.22 The GAB, modified Chung-Pfost, modified Henderson, modified Halsey, and modified Oswin models were adopted as standard equations by the American Society of Agricultural Engineers for describing sorption isotherms (ASAE, 1995).17 The Chung-Pfost, Halsey, Henderson, and Oswin models are rearranged forms of the modified ones, also frequently found in the scientific literature. Among the less common are the Peleg, Sabbah, Copace, Sigma-Copace, Smith and modified Smith models. The Peleg equation is the only one with four parameters in Isotherms and can be used for both sigmoid and non-sigmoid isotherms, performing as well as the GAB model.15 The Smith and modified Smith models are also used in several sigmoid shape isotherms with reliable results,16 as well as the Sabbah, Copace, and Sigma-Copace models.8, 15 In the comparison tests, all simulated isotherms agreed with the values calculated by using electronic worksheets and with the results presented by the literature sources. Future software improvements include the possibility of comparison between different models and/or products, as well as the database expansion.

Conclusion

The Isotherms computational tool was described, providing a free platform for estimating different food sorption curves. From a performance analysis, Isotherms demonstrated its usefulness in the analysis of different sorption models, as well as, of different food hygroscopic behaviors. Additionally, it allows easy database updating and result saving due to the file formats which were considered during its implementation. Isotherms software is a valuable tool to help students, engineers, researchers, and other professionals who work with food water activity and its relationship with industrial processes. The software Isotherms is available on request to the authors. It is free for no-profit use.

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Conflict of interests

Author declares that there is no conflict of interest.

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