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Analytical Methods

Estimation of water activity from pH and °Brix values of some food products

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Abstract

In this study, a predictive model for the estimation of water activity ($a_w^{25\,^\circ C}$) as a function of pH (1.00–8.00) and °Brix (0–82.00) values of simulated food solutions (SFS) was developed, through response surface methodology. Response fit analyses resulted in a highly significant ($pH < 0.0001$) square root polynomial model that can predict $a_w^{25\,^\circ C}$ of SFS in terms of pH and °Brix values within the defined variable ranges. The linear, quadratic and interactive influences of pH and °Brix on $a_w^{25\,^\circ C}$ were all significant ($pH < 0.0001$). Model validations in SFS and in a number of actual food systems showed that the model had acceptable predictive performance, as indicated by the calculated accuracy and bias indices.

Keywords: °Brix; pH; Predictive modelling; Response surface methodology (RSM); Soluble solids; Water activity

1. Introduction

Water activity (a_w) is a measure of the amount of water available for chemical reactions, as well as microbial growth in food (Belitz & Grosch, 1999; Jay, 2000; Rockland & Beuchat, 1987; Troller & Christian, 1978). Furthermore, the mode and severity of food processing for several commodities may be highly dependent on the a_w of the product (Zapsalis, 1985). Therefore, measurement of a_w is essential to the food industry, since it plays a vital role in addressing the needs for product stability, quality maintenance and sustaining the safety of food throughout its shelf-life. Sucrose is a common ingredient of many food products and used as sweetener or a humectant (Triebold & Aurand, 1963; Troller & Christian, 1978). Shelf-life stability of jams, marmalades, fruits in syrups, and other sweetened food products rely on the ability of sucrose to reduce the a_w to a level where microbial growth and unwanted chemical reaction rates are slowed down.

One major factor that influences a_w is the concentration and type of solute present in the food system (Fennema, 1996; Nielsen, 1994). Generally, by simply following Raoult's Law of mole fraction, increase in the amount of solute in a system shall ideally result in a predictable decrease in a_w (Fennema, 1996; Holtzclaw & Robinsons, 1988; Troller & Christian, 1978). Jay (2000), however, cited that many solutes, including the disaccharide sucrose, do not follow Raoult's Law. Interactions of several food properties may possibly explain such a phenomenon. For example, addition of acids in a system containing sucrose causes sugar inversion (Andrews, Godshall, & Moore 2002; Bennion, 1985; McWilliams, 1993). Invert sucrose has been reported to have a greater a_w-lowering effect on foods than sucrose alone (Fennema, 1996).

Despite being one of the more important food parameters that affect food quality and safety, micro- to medium-scale food processors are not able to afford a_w meters. Prices of the least expensive a_w meter models can be as much as US$2000 (Cole-Parmer Instrument Company. Water activity meter systems., 2007; Decagon

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Devices. Water activity for food science: assuring safety & governmental compliance., 2007; Novasina. Water activity: For applications in the food & cosmetic industry., 2007). Furthermore, operation of a_w meters may also be a concern, since stakeholders often lack manpower with sufficient technical knowledge. This study, therefore, tried addressing this gap, by developing a mathematical model capable of predicting the a_w at fixed temperature ($a_w^{25\,°C}$) of some foods, from easily measured, pertinent physicochemical food properties, namely pH and °Brix values. The study established a predictive model in simulated food solutions (SFS), which contained varying levels of water, sucrose and acid. The predictive performance of the established model was assessed through validations using a different set of SFS and various actual food systems.

2. Materials and methods

2.1. Simulated food solutions

The SFS were formulated based on the data supplied to and processed using the Design Expert Version 7.0.3 software package (Statease, Minneapolis, MN). A Central Composite Rotatable Design (CCRD) was applied, to determine the appropriate combinations of various levels of pH and °Brix. Table 1 presents the coded and uncoded SFS formulations that resulted from the CCRD. The assigned °Brix values per SFS were achieved by dissolving food grade D-sucrose (Ajax Finechem, Australia) in de-ionised distilled water. The desired pH value per SFS was adjusted using 5 N HCl (Himedia, Mumbai, India) or 8 N NaOH (Himedia). Freshly prepared solutions were immediately subjected to a_w analyses.

Table 1
Rotatable central composite design used in the formulation of simulated food solutions

Experimental runs[a]	Blocks	Coded variable combinations		Uncoded variable combinations	
		pH	°Brix	pH	°Brix
6	1	0	0	4.50	41.00
5	1	0	0	4.50	41.00
1	1	−1	−1	2.00	12.00
4	1	+1	+1	7.00	70.00
2	1	+1	−1	7.00	12.00
3	1	−1	+1	2.00	70.00
7	1	0	0	4.50	41.00
11	2	0	+α	4.50	82.00
13	2	0	0	4.50	41.00
14	2	0	0	4.50	41.00
8	2	−α	0	1.00	41.00
12	2	0	0	4.50	41.00
9	2	+α	0	8.00	41.00
10	2	0	−α	4.50	0.00

[a] Experimental runs are presented according to the established randomized order of the design of experiment.

2.2. Measurement of a_w

The Novasina™ ms1 set aw (Novasina, Pfaffikon, Switzerland) was used to measure the water activity of the samples at 25 °C ($a_w^{25\,°C}$). Prior to using the device, the instrument was calibrated using saturated salt solutions of known relative humidity (RH) standards namely, 11.3%, 32.8%, 52.9%, 75.3%, and 90.1% RH. After the calibration, 5.0 ml of the sample was placed inside the measuring chamber and the head sensor was fitted to seal the chamber. The $a_w^{25\,°C}$ values were obtained with ±0.01 accuracy. Measurements were done in triplicate.

2.3. Predictive model development and analysis

The general form of the quadratic polynomial model equation used in the study is presented in Eq. (1) (Adinarayana & Ellaiah, 2002; Han, Floros, Linton, Nielsen, & Nelson, 2002). This equation contains linear terms x_1 and x_2, which correspond to the physicochemical properties pH and °Brix, respectively. Square (x_1^2 and x_2^2) and interaction ($x_1 \times x_2$,) terms are also included in the equation. The y value corresponds to the response variable, $a_w^{25\,°C}$, while the β terms are regression coefficients.

$$Y = \beta_0 + \beta_1(x_1) + \beta_2(x_2) + \beta_{1\times 2}(x_1 \times x_2) + \beta_{1\times 1}(x_1^2) + \beta_{2\times 2}(x_2^2) \qquad (1)$$

The $a_w^{25\,°C}$ measured from the test SFS were subjected to response surface model fitting (Adinarayana & Ellaiah, 2002). Data analyses were conducted using the Design Expert Version 7.0.3 (Statease, Minneapolis, MN) software package. The response surface plotted to demonstrate the influences of the predictive variables on the response was constructed using STATISTICA software package, 1999 version (Statsoft, Inc., Tulsa, OK).

2.4. Model validation

The predictive performance of the derived model was validated in a separate set of SFS with pH and °Brix values different from those identified by the CCRD. A number of appropriate actual food systems were also used in validating the performance of the model. Freshly prepared validating SFS with randomly assigned physicochemical properties (Table 5) were subjected to $a_w^{25\,°C}$ analyses following the previously detailed methods. For actual food systems, 5.0 ml or 5.0 g of the food sample was similarly subjected to $a_w^{25\,°C}$ measurement. The pH and °Brix values of the validating SFS and food systems were measured and factored into the developed model to calculate the predicted $a_w^{25\,°C}$ (${}^{p}a_w^{25\,°C}$). The $a_w^{25\,°C}$ values measured by the a_w meter (${}^{a}a_w^{25\,°C}$) were then compared with the ${}^{p}a_w^{25\,°C}$, to assess the predictive performance of the model.

The mathematical predictive model assessments were done by calculating the model performance indices, accuracy factor (A_f) and bias factor (B_f), defined by Ross