Food Research International 45 (2012) 132–135

Contents lists available at SciVerse ScienceDirect

Food Research International

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

Short communication

Modelling the effect of temperature on the lipid solid fat content (SFC)

Pedro E.D. Augusto [a,c,*], Beatriz M.C. Soares [b,c], Ming C. Chiu [c], Lireny A.G. Gonçalves [c]

[a] Technical School of Campinas (COTUCA), University of Campinas (UNICAMP), Campinas, SP, Brazil
[b] Packaging Technology Center (CETEA), Institute of Food Technology (ITAL), Campinas, SP, Brazil
[c] Department of Food Technology (DTA), School of Food Engineering (FEA), University of Campinas (UNICAMP), Campinas, SP, Brazil

ARTICLE INFO

Article history:
Received 24 August 2011
Accepted 18 October 2011

Keywords:
Food properties
Fats
Lipids
Oils
Solid fat content (SFC)

ABSTRACT

The solid fat content (SFC) is an important physical property of lipids, expressing their physical, sensorial, technological and protecting/release properties. In spite of being frequently used, the temperature for a specific SFC is in general obtained by direct interpolation of experimental data, with any modelling and comparison described in literature. The present work evaluated three sigmoidal functions (the Gompertz model, a power decay model and the Logistic model) for modelling the effect of temperature on SFC, using twenty lipids, comprising animal and vegetable native fats and oils, as well as those obtained by interesterification, hydrogenation and/or fractionation. The three models described well the experimental data, with R^2 higher than 0.96. However, the Gompertz model describes it better especially at low and high values of SFC. The results here presented are potentially useful for future studies on lipid technology.

1. Introduction

The solid fat content (SFC) is an important physical property of lipids, which express the solid fraction amount at each temperature. It affects physical properties such as spreadability, consistency and stability, influences important sensorial properties (Ribeiro, Basso, Grimaldi, Gioielli, & Gonçalves, 2009a) and protecting/release properties in encapsulation technology.

Therefore, the SFC is widely used to describe and understand food properties and applications, as well as its behaviour in different storage, processing and consuming conditions. In fact, Flöter (2009) observed that the SFC vs. temperature curve is the predominant parameter to quantify the structuring potential of a fat composition.

In spite of being frequently used, the temperature for a specific SFC is in general obtained by direct linear interpolation of experimental data, with any modelling and comparison described in literature.

The effect of temperature on lipids SFC is described by a characteristic decayed S-shaped curve (Fig. 1) with two asymptotic values. At low temperatures, the SFC tends to a maximum asymptotic value, from which melting starts to decay the solid content. At intermediate temperatures, the SFC decays with an inflexion point. At high temperatures lipid is completed melted, i.e., the SFC tends to a minimum asymptotic value of 0%, as no more solid fat is observed.

Modelling physical properties as a function of process and consuming parameters and conditions is essential for unit operations design, process optimization and high quality products assurance. The present work evaluated three sigmoidal functions for modelling the solid fat content (SFC) of twenty lipids as function of temperature.

2. Materials and methods

Twenty lipids were evaluated, comprising animal and vegetable native fats and oils, as well as those obtained by interesterification, hydrogenation and/or fractionation. Its SFC at each temperature were obtained in literature works (Table 1), using the nuclear magnetic resonance (NMR) method (Farmani, Safari, & Hamedi, 2009; Fatouh, Mahran, El-Ghandour, & Singh, 2007; Grimaldi, Gonçalves, & Esteves, 2000; Nasirullah, Shetty, & Yella, 2010; Shen, Birkett, Augustin, Dungey, & Versteeg, 2001; Singh, McClements, & Marangoni, 2002; Soares et al., 2010; Tarmizi, Siew, & Kuntom, 2008; Wilson & Pease, 1999; Zhang, Pedersen, Kristensen, Nissen, & Holm, 2004) or the differential scanning calorimeter (DSC) method (Khatoon & Reddy, 2005; Li et al., 2010; Reddy & Jeyarani, 2001).

Sigmoidal curves have been extensively used in different areas, describing a wide number of applications. Although many algebraic expressions can represent such curves, only a small number of different functions are frequently encountered (Kaplan & Glass, 1995).

The SFC as function of temperature (T) was modelled using three sigmoidal functions, i.e., the Gompertz model (Eq. (1)), a power decay model (Eq. (2)) and the Logistic model (Eq. (3)). Although many sigmoidal functions are known, the Gompertz and the Logistic models are two of the most used for mathematical modelling. Moreover, the three models here evaluated characterize well the sigmoidal functions, as they are composed by a more direct exponential decay

* Correspondent author at: COTUCA/UNICAMP - Rua Culto à Ciência, 177, Botafogo, CEP: 13020-060, Campinas, SP, Brazil. Tel.: +55 19 3521 9950; fax: +55 19 3521 9998.
E-mail address: pedro@cotuca.unicamp.br (P.E.D. Augusto).

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doi:10.1016/j.foodres.2011.10.026

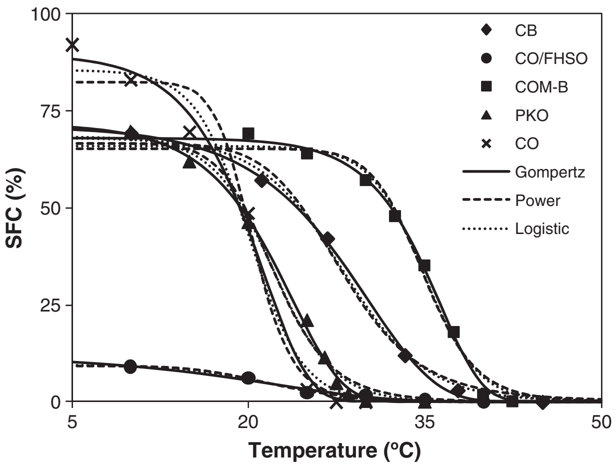

Fig. 1. Example of the effect of temperature on solid fat content (SFC): cocoa butter (CB), chemical interesterification of canola oil and fully hydrogenated soybean oil (CO/FHSO), commercial bakery fat (COM-B) and palm kernel oil (PKO). Markers are the experimental values; curves are the Gompertz model (Eq. (1)), the power sigmoidal model (Eq. (2)) and the Logistic model (Eq. (3)).

(Eq. (3)), a power decay (Eq. (2)) and a more complex-exponential decay (Eq. (1)).

$$\mathrm{SFC}(\%) = a \cdot e^{-e^{(b - c \cdot T)}} \tag{1}$$

$$\mathrm{SFC}(\%) = \frac{a}{1 + (b \cdot T)^c} \tag{2}$$

$$\mathrm{SFC}(\%) = \frac{a}{1 + b \cdot e^{c \cdot T}} \tag{3}$$

The goodness of the models was evaluated by plotting the values of SFC obtained by models ($\mathrm{SFC}_{\mathrm{model}}$) as a function of the experimental values ($\mathrm{SFC}_{\mathrm{experimental}}$). The regression of those data to a linear function (Eq. (4)) results in three parameters that can be used to evaluate the description of the experimental values by the models, i.e. the linear slope (α; that must be as close as possible to the unit), the intercept (β; that must be as close as possible to zero) and the coefficient of determination (R^2; that must be as close as possible to the unit). It is a simple and efficient approach to evaluate the model fit (Augusto et al., in press). Moreover, the values to the R^2 of regression to Eqs. (1)–(3), residual sum of squares (RSS, Eq. (5)) and the mean residual sum of squares (MRSS, Eq. (6)) were used in order to evaluate the model fit.

$$\mathrm{SFC}_{\mathrm{model}} = \alpha \cdot \mathrm{SFC}_{\mathrm{experimental}} + \beta \tag{4}$$

$$\mathrm{RSS} = \sum_{i=1}^{n} \left(\mathrm{SFC}_{\mathrm{experimental}} - \mathrm{SFC}_{\mathrm{model}} \right)_i^2 \tag{5}$$

$$\mathrm{MRSS} = \frac{\mathrm{RSS}}{n} \tag{6}$$

The parameters of each model were obtained by non-linear regression using CurveExpert Professional 1.2.3 software, considering a significant probability level of 95%.

3. Results and discussion

Table 2 shows the obtained parameters for the Gompertz (Eq. (1)), the power decay sigmoidal (Eq. (2)) and the Logistic (Eq. (3)) models. The model regressions showed high values for the coefficient of determination ($R^2 > 0.96$), as well as suitable levels for the RSS and MRSS values (Table 3).

Eq. (4) was used in order to evaluate the efficiency of each model in describe the experimental values. The parameters α, β and R^2 are shown in Table 3. For the Gompertz model, α values were between 0.97 and 1.12, β between −2.73 and 1.16, and R^2 between 0.97 and 1.00. For the power decay sigmoidal model, α values were between 0.92 and 0.99, β between 0.01 and 3.49, and R^2 between 0.97 and 0.99. For the Logistic model, α ranged between 0.94 and 1.01, β between −1.09 and 3.04, and R^2 between 0.97 and 1.00. The obtained results indicate that the three models describe well the experimental data and that the evaluated sigmoidal functions can be used for modelling the effect of temperature on lipids solid fat content (SFC).

Moreover, the Gompertz model described experimental values slightly better than the power decay sigmoidal and Logistic models (Tables 2 and 3). It can be graphically seen in Figs. 1 and 2. The Gompertz model better suits the SFC data especially at low solid content (where the other two models tend to overestimate the SFC value) and at high solid content (where the other models tend to underestimate the SFC).

In spite of being a frequently used property, the SFC is generally used as a qualitative tool in lipid evaluation, and its relation with

Table 1
The twenty evaluated lipids.

Lipid	Description	Source
AMF	Anhydrous milk fat	Singh et al. (2002)
BBO	Buffalo butter oil	Fatouh et al. (2007)
MF	Mango fat	Reddy and Jeyarani (2001)
PO	Palm oil	Tarmizi et al. (2008)
S-PO	Stearin – palm oil	Tarmizi et al. (2008)
O-PO	Olein – palm oil	Tarmizi et al. (2008)
PKO	Palm kernel oil	Soares et al. (2010)
S-PKO	Stearin – palm kernel oil	Soares et al. (2010)
O-PKO	Olein – palm kernel oil	Soares et al. (2010)
PS/CO	Enzymatic interesterification of palm stearin and coconut oil	Zhang et al. (2004)
SO/FHSO	Enzymatic interesterification of soybean oil and fully hydrogenated soybean oil	Zhang et al. (2004)
HO/FHSO	Enzymatic interesterification of high oleic sunflower oil and fully hydrogenated soybean oil	Li et al. (2010)
CO/O-PO	Chemical interesterification of canola oil and palm olein	Farmani et al. (2009)
CO/FHSO	Chemical interesterification of canola oil and fully hydrogenated soybean oil	Farmani et al. (2009)
COM-B	Commercial bakery fat	Khatoon and Reddy (2005)
COM-SH	Commercial shortening	Khatoon and Reddy (2005)
COM-SO	Commercial soup fat	Grimaldi et al. (2000)
CO	Coconut oil	Nasirullah et al. (2010)
CB	Cocoa butter	Wilson and Pease (1999)
HCO	Hydrogenated coconut oil	Shen et al. (2001)