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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

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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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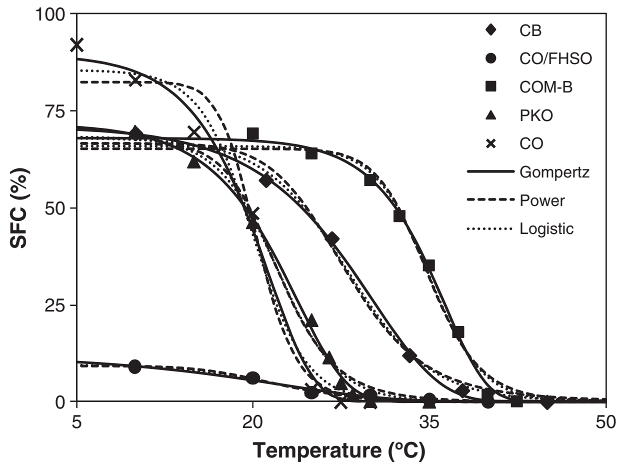

Fig. 1. Example of the effect of temperature on solid fat content (SFC): cocoa butter (CB), chemical interesterification of canola oil and fully hydrogenated soybean oil (CO/FHSO), commercial bakery fat (COM-B) and palm kernel oil (PKO). Markers are the experimental values; curves are the Gompertz model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

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

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

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

The goodness of the models was evaluated by plotting the values of SFC obtained by models ($\text{SFC}_{\text{model}}$) as a function of the experimental values ($\text{SFC}_{\text{experimental}}$). 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.

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

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

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

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)

Table 2
Values for the parameters of the Gompertz (Eq. (1)), power sigmoidal (Eq. (2)) and Logistic (Eq. (3)) models (T = temperature in °C).

Lipid	Gompertz $SFC(\%) = a \cdot e^{-e^{(b-c\cdot T)}}$			Sigmoidal – power $SFC(\%) = \frac{a}{1+(b\cdot T)^c}$			Logistic $SFC(\%) = \frac{a}{1+b\cdot e^{c\cdot T}}$		
	a	*b*	*c*	*a*	*b*	*c*	*a*	*b*	*c*
AMF	47.76	−2.978	−0.203	41.01	0.075	5.266	43.19	0.008	0.357
BBO	80.89	−0.418	−0.051	39.70	0.071	2.591	51.53	0.244	0.128
MF	90.57	−7.203	−0.239	86.27	0.035	11.05	88.00	$3.3 \cdot 10^{-5}$	0.364
PO	101.1	−1.084	−0.070	70.35	0.064	3.057	79.14	0.108	0.152
S-PO	195.7	−0.323	−0.037	70.81	0.044	3.465	85.86	0.089	0.118
O-PO	73.48	−2.328	−0.163	65.98	0.081	4.136	68.04	0.027	0.289
PKO	71.54	−5.559	−0.234	66.67	0.045	9.298	68.18	$1.9 \cdot 10^{-4}$	0.389
S-PKO	75.98	−6.422	−0.241	71.83	0.040	10.10	73.27	$7.8 \cdot 10^{-5}$	0.375
O-PKO	72.81	−5.053	−0.229	65.50	0.048	9.995	67.54	$1.6 \cdot 10^{-4}$	0.424
PS/CO	131.6	−1.193	−0.059	78.67	0.044	3.995	93.52	0.060	0.135
SO/FHSO	56.85	−0.706	−0.039	28.85	0.039	3.061	37.43	0.148	0.090
HO/FHSO	89.62	−2.074	−0.060	68.16	0.030	4.420	76.26	0.029	0.112
CO/O-PO	96.78	−0.178	−0.047	27.10	0.053	4.355	36.86	0.092	0.158
CO/FHSO	11.88	−2.389	−0.106	9.105	0.045	6.277	9.600	0.005	0.241
COM-B	68.06	−10.24	−0.282	65.35	0.029	15.85	66.02	$2.1 \cdot 10^{-7}$	0.440
COM-SH	62.39	−6.864	−0.186	58.13	0.028	10.98	59.25	$2.6 \cdot 10^{-5}$	0.301
COM-SO	80.73	−4.051	−0.109	71.12	0.029	7.322	75.07	0.002	0.183
CO	89.46	−5.580	−0.261	82.49	0.049	12.33	85.52	$1.4 \cdot 10^{-4}$	0.443
CB	70.92	−5.226	−0.173	66.47	0.036	8.465	68.10	$3.9 \cdot 10^{-4}$	0.280
HCO	101.9	−3.751	−0.154	97.15	0.047	5.936	98.71	0.004	0.259

temperature is mainly graphically (i.e., qualitatively) evaluated. One example is the descriptive evaluation of the effect of interesterification on the lipid SFC shape (see, for example, Ribeiro, Grimaldi, Gioielli, & Gonçalves, 2009b). A mathematical description of SFC curve is highly desirable in order to enable an objective evaluation.

Furthermore, a quantitative interpretation is often necessary for product and process design, as the SFC correspondent of a specific temperature or the temperature when it is observed a specific SFC. This information is in general obtained by direct linear interpolation between two experimental data or, moreover, by approximating the SFC vs. temperature curve using polynomial functions.

The polynomial function adjustment approach is commonly used for melting point calculation, i.e., the temperature corresponding to the SFC of 4% (Karabulut, Turan, & Ergin, 2004; Ribeiro et al., 2009a; Ribeiro et al., 2009b).

Ospina-E, Cruz-S, Pérez-Álvarez, and Fernández-López (2010) used a polynomial function for modelling the relation between pork fat SFC and temperature and the stearic acid content (C18:0). The effect of temperature on the SFC was described by a second-order (quadratic) polynomial function.

Apparently, the use of polynomial functions can well describe the SFC experimental data, sometimes with high coefficient of determination. An example can be seen for the commercial bakery fat (COM-B) and mango fat (MG) in Fig. 2, where a second-order (quadratic) polynomial function was adjusted to the experimental data with $R^2 = 0.97$ and 0.93, respectively.

However, it is important to notice that the polynomials' functions are not suitable for representing the S-shape of the SFC vs. temperature curve, and that high correlation can only be obtained when just an intermediate part of the curve is evaluated. It is clear in Fig. 2, where the two asymptotic regions cannot be correctly described. Thus, we highlight the importance of using sigmoidal functions to describe the lipids SFC.

The obtained results indicate that the three functions here evaluated can be used for modelling the effect of temperature on lipids solid fat content (SFC). The models here described can be used to evaluate the effect of processing technologies and conditions on the lipid SFC.

Table 3
Evaluation of the obtained models.

Lipid	Gompertz Eq. (1)			Eq. (4)			Sigmoidal – power Eq. (2)			Eq. (4)			Logistic Eq. (3)			Eq. (4)		
	R^2	RSS	MRSS	α	β	R^2	R^2	RSS	MRSS	α	β	R^2	R^2	RSS	MRSS	α	β	R^2
AMF	1.00	0.10	0.01	1.00	0.02	1.00	0.99	14.08	1.76	0.97	0.70	0.99	1.00	4.70	0.59	0.99	0.31	1.00
BBO	1.00	7.72	0.86	0.99	1.19	1.00	0.98	22.94	2.55	0.96	1.03	0.99	1.00	8.09	0.90	0.98	0.43	1.00
MF	0.99	134.1	16.76	0.98	0.77	0.99	0.97	316.3	39.54	0.94	3.25	0.97	0.98	252.5	31.57	0.95	2.77	0.98
PO	1.00	20.32	2.54	1.01	−0.62	1.00	1.00	15.93	1.99	0.98	0.88	1.00	1.00	3.43	0.43	1.00	−0.12	1.00
S-PO	1.00	290.8	32.31	1.13	−2.73	0.98	1.00	57.15	6.35	0.94	1.35	0.99	1.00	7.10	0.79	1.01	−0.37	1.00
O-PO	1.00	4.84	0.97	1.01	−0.65	1.00	1.00	11.00	2.20	0.98	0.98	1.00	1.00	0.38	0.08	1.00	0.20	1.00
PKO	1.00	14.17	1.57	0.99	0.43	1.00	0.99	84.30	8.37	0.96	1.89	0.99	0.99	56.57	6.29	0.97	1.24	0.99
S-PKO	1.00	9.52	1.06	1.00	0.22	1.00	0.99	77.88	8.65	0.96	1.81	0.99	0.99	48.00	5.33	0.97	1.31	0.99
O-PKO	1.00	13.44	1.49	0.99	0.48	1.00	0.99	68.33	7.65	0.97	1.21	0.99	0.99	46.57	5.17	0.98	1.09	0.99
PS/CO	1.00	1.19	0.24	1.00	0.08	1.00	1.00	15.49	3.10	0.99	0.74	1.00	1.00	6.11	1.22	0.99	0.45	1.00
SO/FHSO	1.00	0.36	0.07	1.00	−0.01	1.00	1.00	0.27	0.05	1.00	0.07	1.00	1.00	0.19	0.04	1.00	0.00	1.00
HO/FHSO	0.99	67.94	6.18	0.97	1.16	0.99	0.97	238.6	21.69	0.93	3.30	0.97	0.98	135.8	12.34	0.95	2.33	0.98
CO/O-PO	1.00	0.27	0.04	1.00	0.06	1.00	1.00	1.55	0.26	0.99	0.23	1.00	1.00	0.70	0.12	0.99	0.15	1.00
CO/FHSO	0.98	1.25	0.21	0.99	−0.01	0.98	0.99	0.58	0.10	0.99	0.02	0.99	0.99	0.79	0.13	1.00	0.02	0.99
COM-B	1.00	10.97	1.37	0.99	0.60	1.00	0.99	68.83	8.60	0.95	2.26	0.99	0.99	51.62	6.45	0.96	1.98	0.99
COM-SH	1.00	13.66	1.71	0.99	0.37	1.00	0.99	31.08	3.89	0.97	1.20	0.99	0.99	23.21	2.90	0.98	0.97	0.99
COM-SO	0.99	67.13	8.39	0.98	1.23	0.99	1.00	208.1	26.01	0.93	3.50	0.97	0.98	137.1	17.17	0.94	2.88	0.98
CO	0.99	69.53	9.93	0.98	1.15	0.99	0.98	235.4	33.63	0.96	2.60	0.98	0.98	175.4	25.06	0.95	3.04	0.98
CB	1.00	3.64	0.61	1.00	−0.26	1.00	0.99	31.52	5.25	0.97	1.26	0.99	1.00	13.19	2.20	0.99	0.74	1.00
HCO	0.99	60.73	10.12	1.02	−2.18	1.00	1.00	3.40	0.57	1.00	0.12	1.00	1.00	11.99	2.00	1.01	−1.10	1.00

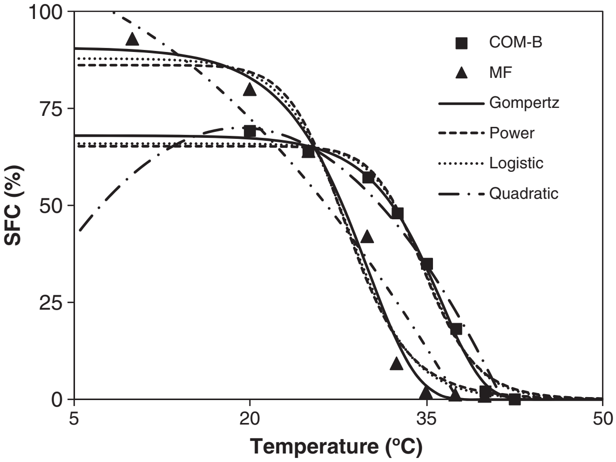

Fig. 2. Example of the effect of temperature on solid fat content (SFC) for the commercial bakery fat (COM-B). Markers are the experimental values; curves are the Gompertz model (Eq. (1)), the power sigmoidal model (Eq. (2)), the Logistic model (Eq. (3)) and the second-order polynomial (quadratic) function.

Moreover, it can be directly used for better estimate the temperature correspondent to a specific SFC (which is important, for example, for determining the lipids melting point), as well as intermediate values between experimental points (using suitable non-linear interpolation). By mathematically describing this important lipid property, different lipid products and processing can be better evaluated and designed in an objective way.

4. Conclusions

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 solid fat content (SFC), considering twenty lipids. Although the three models described well the experimental data, the Gompertz model described it better at low and high values of SFC. As there is any work in literature modelling the SFC curve, the mathematical description of this important lipid property enable products and processing better evaluation and design in an objective way. The results presented here are potentially useful for future studies on lipid technology.

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