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Solid Fat Content of vegetable oils and simulation of interesterification reaction: Predictions from thermodynamic approach

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ABSTRACT

The Solid Fat Content (SFC) of vegetable oils is a fundamental property in fatty foods. Also, chemical interesterification (the exchange of fatty acids within and between triacylglycerols) has been used to enhance the melting profile of vegetable oils blends used in food industry. The present work uses a computational approach using Solid–Liquid Equilibrium (SLE) to predict SFC and simulate the chemical interesterification reaction (CI) for different formulations using palm oil (PO), sunflower oil (SFO) and palm kernel oil (PKO). More than 3696 SLE problems are solved, allowing the evaluation of how the fraction of each oil, the temperature and the CI reaction impacts the SFC. The calculated SFC values are compared with experimental data taken from literature. For systems composed of two or one single vegetable oil, the average absolute error (AAE) is 5.2% before CI and 4.2% after CI. For systems composed of three vegetable oils, the AAE is 6.3% before CI and 4.2% after CI. The predictions of SFC before and after CI reaction can aid the food makers to face the combinatorial problem imposed by the choice of the vegetable oil and its fraction in the blend. Future improvements in the pure component properties, thermodynamic model and distribution model of fatty acids in the triacylglycerols can increase the use of computational approaches allowing the experiments to be focused on the most promising formulations in terms of melting profile.

1. Introduction

The Solid Fat Content (SFC) of a vegetable oil blend is responsible for many fundamental characteristics of fatty foods, such as physical appearance, organoleptic properties and spreadability, also influencing plasticity of an edible oil product (Rao et al., 2001). Some attempts to compute SFC and other melting-related properties of vegetable oils (VOs) can be found in the literature. Most of them use non-phenomelogical methods, such as neural networks (Block et al., 1997) and empirical correlations regressing experimental data (Augusto et al., 2012; Fasina et al., 2008; Soares et al., 2009). Thermodynamic approaches are still scarce. The modeling of the Solid–Liquid Equilibrium (SLE) problem in systems composed by fatty acids and triacylglycerols can be found in the works of Boodhoo et al. (2008), Rocha and Guirardello (2009), Wesdorp et al. (2005) and Won (1993). Recently, we have showed how computational tools are useful in predicting SFC of binary blends of VOs, with and without interesterification (Teles dos Santos et al., 2013). The aim of the present work is further compare predicted values of SFC with experimental data and highlight how modeling and simulation can help product design of fatty products matching a desired melting profile.

2. Solid Fat Content

Fig. 1 shows the variables affecting consumers' perception of fat-based foods. It can be noted that many issues contribute to the desired attributes on the final product. The "missing link" corresponds to factors that influence the sensorial perception of food texture (Engelen and Van der Bilt, 2008).

Despite the multiple interactions between these factors, some direct correlations between SFC and desired attributes are established. Some examples gathered from literature are (Arifin et al., 2009; Criado et al., 2008; Lida and Ali, 1998; Osborn and Akoh, 2002; Torbica et al., 2006):

- The SFC between 4 °C and 10 °C determines the ease of spreading of the product at refrigeration temperature and a value not greater than 32% at 10 °C is essential for good spreadability.
- The SFC at 20 °C and 22 °C determines the product's stability and resistance to oil exudation at room temperature.

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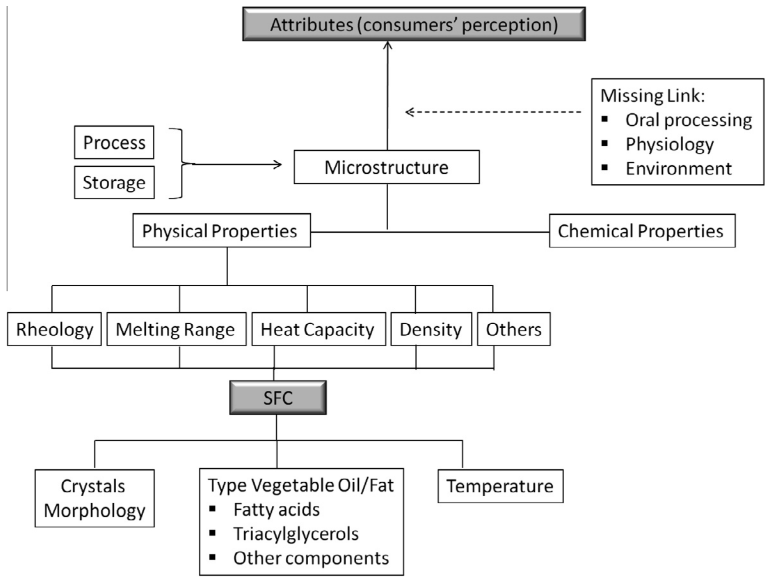

Fig. 1. From fundamental variables to consumers' desired attributes: the role of Solid Fat Content.

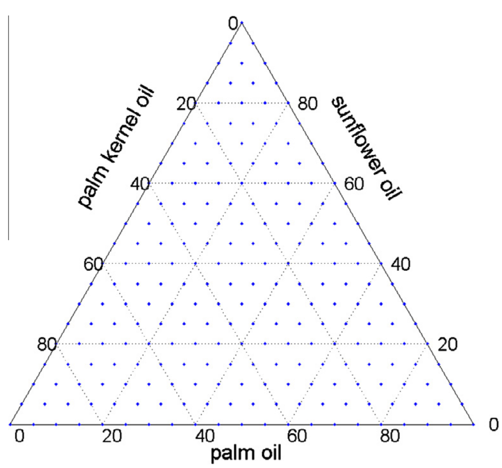

Fig. 2. Ternary diagram with 231 points in which the Solid–liquid Equilibrium problem is solved. Blend PO–SFO–PKO.

- A value of not less than 10% is essential to prevent oiling off.
- The SFC between 35 °C and 37 °C determines the thickness and flavor release.
- Margarines without a waxy mouth feel have a SFC less than 3.5% at 33.3 °C and melt completely at body temperature. A large difference between the SFC at 15 °C and 25 °C is correlated to cooling sensations.
- In baking shortenings, optimal performance is achieved with a SFC between 15% and 25% at the usage temperature whereas an excess of liquid can cause an oiliness sensation decreasing scores of sensorial attributes.
- The temperature range within a fat can retain its consistency is determined by the temperatures within the SFC values lie in the range 15–35%.
- At the range 33–38 °C, the SFC values influence the "mouth feel" or waxy sensations that are induced by the fat.
- The SFC profile of cocoa butter substitutes must have a sharp decrease in solid fat near body temperature as in natural cocoa butter. SFC below 25 °C characterize its hardness, while SFC between 25 °C and 30 °C indicates the

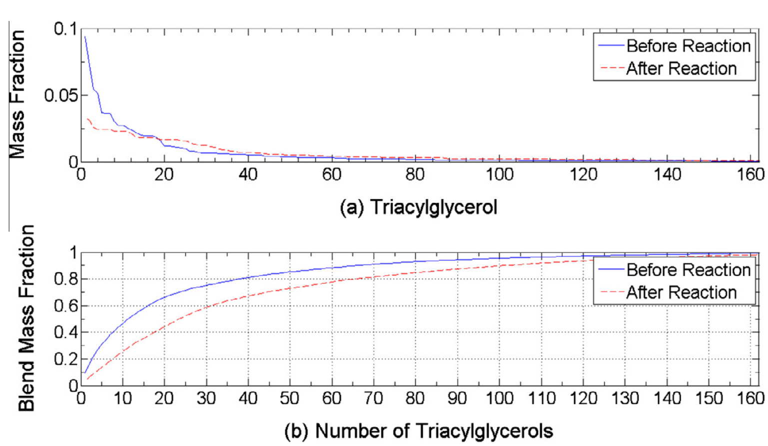

Fig. 3. (a) Calculated mass fraction of each TAG present in the blend PO–SFO–PKO (1–1–1) before and after reaction. (b) Number of TAGs and corresponding mass fraction of the blend PO–SFO–PKO (1–1–1) before and after reaction.