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VIS–NIR spectroscopy as a process analytical technology for compositional characterization of film biopolymers and correlation with their mechanical properties

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ABSTRACT

There is an increasing interest in the use of polysaccharides and proteins for the production of biodegradable films. Visible and near-infrared (VIS–NIR) spectroscopy is a reliable analytical tool for objective analyses of biological sample attributes. The objective is to investigate the potential of VIS–NIR spectroscopy as a process analytical technology for compositional characterization of biodegradable materials and correlation to their mechanical properties. Biofilms were produced by single-screw extrusion with different combinations of polybutylene adipate-co-terephthalate, whole oat flour, glycerol, magnesium stearate, and citric acid. Spectral data were recorded in the range of 400–2498 nm at 2 nm intervals. Partial least square regression was used to investigate the correlation between spectral information and mechanical properties. Results show that spectral information is influenced by the major constituent components, as they are clustered according to polybutylene adipate-co-terephthalate content. Results for regression models using the spectral information as predictor of tensile properties achieved satisfactory results, with coefficients of prediction (R^2_C) of 0.83, 0.88 and 0.92 (calibration models) for elongation, tensile strength, and Young's modulus, respectively. Results corroborate the correlation of NIR spectra with tensile properties, showing that NIR spectroscopy has potential as a rapid analytical technology for non-destructive assessment of the mechanical properties of the films.

1. Introduction

Plastic materials present several advantages such as being chemically and mechanically resistant, lightweight, heat-sealable, can be printed on and are available in large quantities at low cost, thus been widely used as food packaging. However, synthetic plastic materials are derived from non-renewable sources such as petroleum, and most of them are not biodegradable. Thus, they are environmentally harmful and their use has been restricted to avoid ecological damages [1]. The problems caused by discarding non-biodegradable materials have led to the research and development of biodegradable materials with characteristics that allow for their use in the production of packaging on a commercial scale. Biopolymers such as polysaccharides and proteins are available in large amounts from renewable sources [2]. There is an increasing interest in the use of biopolymers that could minimize the environmental impact of synthetic plastics. Starch-based materials stand out among the ones obtained from renewable sources, being used in the production of biodegradable materials such as films and sheets [3]. However, the drawbacks of starch-based materials include poor mechanical properties and high hydrophilicity. Several studies have proposed the addition of protein, fiber, or lipids to improve these properties but they were unable to achieve satisfactory results.

Determination of mechanical properties of film polymers requires destructive and time consuming methods, and is carried out in specific equipment such as texturometers by specialized analysts [4,5]. Thus, large scale production of films requires fast and non-invasive analytical methods in order to assess film composition and mechanical properties. Visible and near-infrared (VIS–NIR) spectroscopy is a well-established alternative as a non-destructive process analytical technology for measuring constituents of biological materials. The NIR spectrum is influenced by the different vibrational modes of the molecules, which are caused by their interaction with electromagnetic radiation absorbed at specific wavelengths. This technique has been used for the identification of several complex components such as proteins and carbohydrates in biological materials. Chemometrics allows the extraction of relevant information contained in the spectra for the development of calibration

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