Abstract

Direct calculation of amylose-amylopection ratios and other proximates by curve fitting of near infrared spectra of cereal flours

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Introduction

Amylose, protein and fibre content of grains are important factors for cereal flour quality. While NIR spectroscopic determinations of these attributes by means of multivariate analysis are widely reported, they all require large sets of samples and multiple models for different types of cereals. A direct calculation of these parameters based on NIR spectra of reference materials can be an attractive method because, in its simplest form, there is no calibration, does not require linkage with a specific set of samples and can be extended to different instruments without the need for standardisation. In this study, based on methods reported in the literature, a direct calculation of moisture, fat, protein, amylose and total fibre content of rice, wheat and corn flours was performed by means of a non-negative least squares algorithm. The technique attempts a curve fitting of a cereal flour NIR spectra with a sum of the spectra of reference materials. Good agreement has been found between the calculated parameters and values from reference methods (Table 1).

Materials and methods

The reference materials used are: pure amylose from potato, pure corn amylopectin, corn oil, water, wheat gluten, wheat gliadin, arabinoxylan, and gelatinised corn amylopectin, all available

Table 1. Fit goodness and correlation with reference values for NIR direct calculation of cereal flours.

	Rice Flour	Wheat Flour	Corn Flour
% Explained flour NIR spectrum	99	98	98
R2 Amylose	0.95	0.96	0.96
R2 Proteins	0.96	0.97	0.97
R2 Fibres	0.86	0.94	0.93

commercially. Cereal samples consisted of 90 rice, 110 wheat, and 30 corn flours for which reference values were available. Samples and reference NIR reflectance spectra were acquired between 1100 and 2500 nm with a 2 nm gap on a 6500 NIRSystems scanning monochromator spectrometer (FOSS NIRSystems, Silver Springs, MD, USA). Data was exported as a text file and all spectral pretreatment and processing were performed using in-house developed scripts under Matlab (Mathworks, MA, USA). Spectral pretreatment consisted on the Savitzky-Golay 1st and 2nd derivative followed by a standard normal variate transform.

Model Formulation

Based on the technique described by I.J. Wesley *et al*[1] the model solves a system of n equations with the unknowns c_1 to c_7 which, in matrix notation takes the form $\mathbf{R}^*\mathbf{c}=\mathbf{S}$ where n are the frequencies at which the NIR measurements are performed, c_i, i = 1,2,..7, are the proportions of each reference material, **R** is a matrix of the NIR spectra of the reference materials and **S** is the NIR measurement of the sample to be evaluated. The solution, in the least squares of this overdetermined system, is given by $\mathbf{c}=\mathbf{R}\backslash\mathbf{S}$.

Results and discussion

The direct calculation relies on the assumption that the sample spectrum is a linear combination of the component spectra and is based on the fact that PLS and PCA rely also on linear variations. This assumption seems to be verified since, with the reference materials chosen here, a good reconstruction

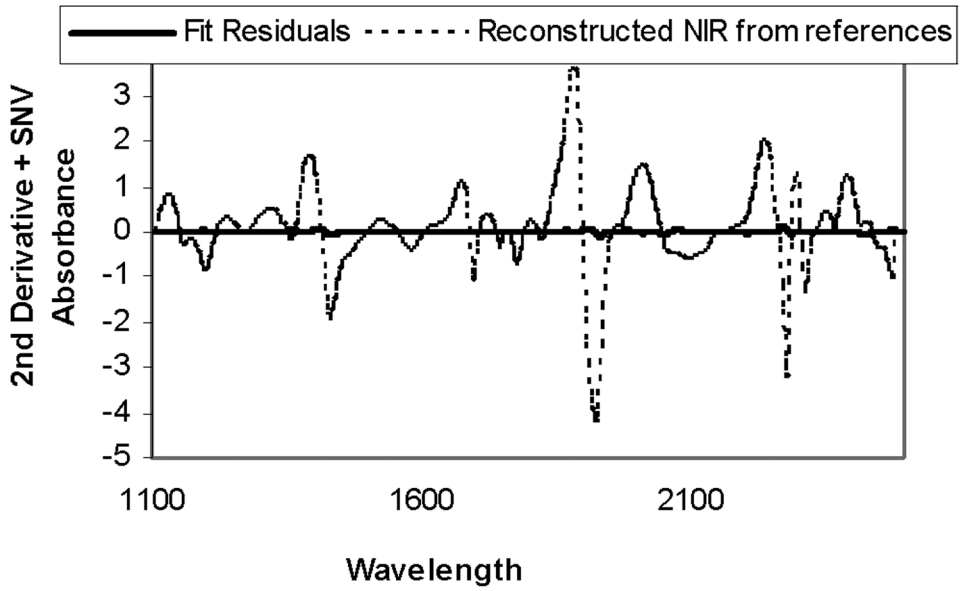

Figure 1. Typical NIR rice flour reconstructed from NIR of reference materials with the resulting residuals.

of the cereal flours NIR spectrum is possible with an average explained variation of 98% based on the ratio of standard deviation of curve fit residuals to standard deviation of the sample NIR spectra, as exemplified in Figure 1 and Table 1.

The gelatinised pure amylopectin gives as well an indication of the flour degree of gelatinisation. This technique also opens up the possibility for quick assessment of the starch morphology in products based on extruded or roller dried cereal flour without need of a prior product specific calibration.

Reference

1. I.J. Wesley, S. Uthayakumaran, R.S. Anderssen, G.B. Cornish, F. Bekes, B.G. Osborne and J.H. Skerrit, *J. Near Infrared Spectrosc.* **7,** 229–440 (1999).