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Temperature Dependent NIR Spectroscopic Analysis for Food Grain Samples

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Abstract

The use of NIR spectroscopy as a tool for sample analysis of food and vegetables is in focus. Shimadzu NIR spectrophotometer is used to get the spectral response of wheat and rice flour. The rice and wheat flour samples were exposed to different temperatures in sample chamber, unlike conventional constant sample temperature. Peak at particular wavelength represents the content and magnitude of peak reflects its concentration. The spectral response reflects change in the peak value which results in error while analyzing the content value. Design of a compensator tool based on data look up technique can cope up analytical error due to temperature change.

Keywords: Food Grain, NIR Spectroscopy, Temperature Dependency

1. Introduction

As a well-known fact, all chemical substance has its unique orbital signature based on its energy band diagram. The atoms shifts from lower to higher or higher to lower energy band is supported by either absorption or emission of equivalent energy as the band gap difference respectively. Most NIR absorption are due to combinational band or first and second overtone vibrations of atoms. Any transfer of atom from n to n+2 is first overtone and n+3 is second overtone combination. The relationship of band gap energy difference to the wavelength in case of food having multi-variate content falls under NIR region. NIR spectral range is 780 nm to 2500 nm. Near infrared reflectance technology is the most practicable and exciting analytical tool to hit the agriculture and food industries since Johan Kjeldah introduced Kjeldah test accepted by Association of American Cereals and Chemist (AACC) as a recommended procedure for Protein content analysis. Kjeldah test comprising of digestion, neutralization and titration stages for protein determination consumes considerable time for content analysis. NIR spectroscopy offers on-line chemometrics solution to such determination by virtue of no sample preparation time and quick analysis of content.

1.1 Sources of Errors in NIR Spectroscopy

NIR method of content analysis is a referenced method as it requires prior knowledge of content concentration. A very well-known Beer Lambert law suggests that the amount of absorption at a particular wavelength is directly proportional to its concentration in a sample. In case of NIR spectroscopy, a sample chamber containing sample is exposed to NIR light at different wavelengths and transmittance is measured at each wavelength. Transmittance as reciprocal of absorption gives the % concentration of a particular substance. Any error in measurement of transmittance will lead to erroneous result in analysis. Error is defined as differences between computed or measured value and the true or correct value. The accepted method of expressing accuracy in classical chemical analysis is in terms of comparison with analysis of known calculated chemical constitution and by spiking the samples with known amount of pure substance and determining the recovery. Expression of accuracy in this manner is difficult

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in NIR analysis. Near infrared reflectance spectroscopy is applied to testing of constituents such as moisture, protein, oil, starch, fibre components and other organic substances of simple and complex nature. The most common method for expressing the accuracy is in terms of Standard Deviation of Differences (SDD) between NIR and standard analysis of unknown samples and by use of check samples, which have been analyzed by standard chemical methods to a degree that establishes confidence in their composition.

Noise in connection with any type of spectroscopy is defined as any disturbance, especially a randomly distributed and persistent disturbance that influences the quality and clarity the electrical signals. The efficiency of an NIR spectrophotometer is markedly affected by the ratio of the electronic signal to the noise. Referred to as SNR (Signal to Noise Ratio) this must be as high as possible. There are main two types of instrument noise; a noise that affects the instrument output on a standard background, such as an optically flat standard and noise caused by interaction between instrument and sample.

A preliminary experimental setup by P.C.Williams at Grain research laboratory, Canadian grain Commission, Winnipeg, Monitoba, Canada has brought to the forefront significance of grinding wheat. The experiment proved that the method of grinding wheat has also significant role in analytical part. If not properly calculated, method of grinding can be a major source of error. Table1 reflects sources of errors in NIR chemometrics need to be addressed to validate the NIR results over and over.

Table 1. Sources of errors in Near Infrared Reflectance testing

Error source	Factors contributing error
Instrument factor	• Instrument noise • Nonlinearity of signal • Wavelength selection • Mathematical treatment of raw log(1/R) data • Derivative size • Static electricity • Instrument temperature control • Power supply fluctuations • Cell windows and aging of components
Sample factors	• Bulk density of ground samples • Physical texture of sample • Sample temperature • Chemical composition • Ambient temperature • Conversion factors
Operational factors	• Calibration practice • Wavelength selection • Sample preparation including grinder type, condition of grinder, mean particle size, blending after grinding etc. • Sample cell loading • Chemical or physiochemical analysis

2. Sample Temperature Dependency on NIR Result

Various sources of errors in NIR spectroscopy has been under study. In this experiment, the main focus was to check the temperature dependencies of sample in NIR spectroscopy. To validate the fact that even if all sources of errors in NIR would have been addressed, the significance of sample temperature on NIR spectral response, Shimadzu make UV-VIS-NIR spectrophotometer at Central Salt Marine Chemical Research Institute, Bhavnagar, Gujarat was used. The sample of wheat and rice flour with known multi-variate content in powder form was under investigation with varying temperature values.

Wheat and rice flour in the powder form with known contents were under investigation. The plotting of datum line based on the sample was an important task for which various compound mixtures were applied as reference sample and Barium oxide was selected as it does not exhibit fluctuations in the datum line in NIR range. Separately wheat/rice flour was exposed to NIR range of 800–2500 nm wavelength spectra and temperature induced variation was applied to the samples. The objective of the experimental set up was to establish temperature dependencies of peak absorbance value. The main issue to address the objective was first to check whether the process of raising the temperature has any effect on the loss of content due to which the peak value change occurs. To check whether the process of heating and then cooling down the sample is a reversible process and content is a recoverable or not, normal temperature spectra were recorded for both the samples. The samples were then exposed to higher temperatures in the oven having temperature range set up at 100°Celsius. The spectra were recorded for three different temperatures which was not measurable using the SPM. The spectra were recorded in both the direction of heating as well as cooling down the sample. Out of 6 peaks recorded from the spectra, peaks repeating itself, were identified and recoverable and reversible content check was ensured.

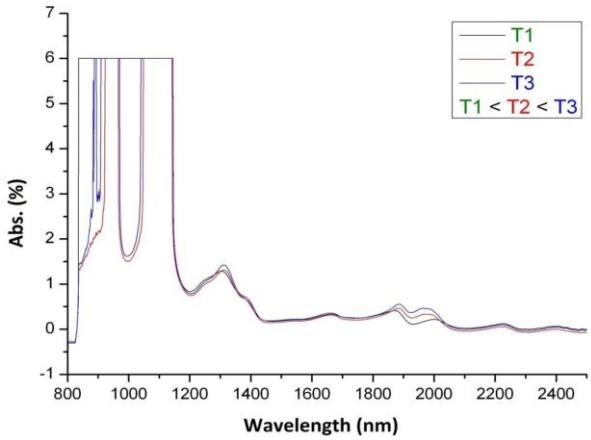

Figure 1. NIR spectra for wheat flourat different temperature.

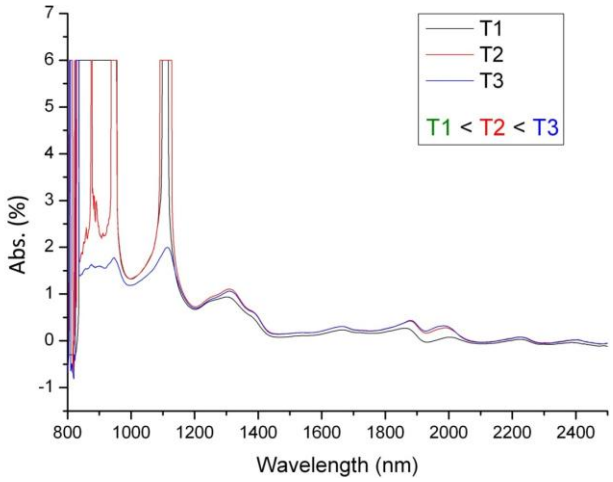

Figure 2. NIR spectra for rice flour at different temperature.

The conclusion derived from spectral response yields two observations. One being presence of particular content based on peak value at particular wavelength and other being % concentration of that compound. As Beer Lambert law suggest that the peak absorbance value depends upon the concentration of that substance and any change due to either instrument error or temperature variation will result in error in predicting the concentration value of that substance. For recoverable content and reversible process, the calculated value of substance shall remain unchanged but due to temperature variations, if not corrected, error in calculation remains.

The peak values for wheat flour at wavelengths 1313, 1883 and 1967 and for rice flour wavelengths at 1311, 1887 and 1971 were repetitive and recoverable content check was established. The experiment has established the sample temperature dependency and NIR spectral response.

3. Conclusion

The NIR spectral response being temperature dependent and variation in the sample temperature if not corrected results in analytical error. Hence need for some compensator is essential to cope up the effect of temperature induced errors on NIR spectral response.

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