

Near Infrared Spectroscopy: a substitute technology over chemical analysis techniques : A review for food industries

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Abstract— This paper focuses on potential capacity of Near Infrared Spectroscopy as an online real time component analysis techniques over conventional chemical analysis techniques. The acceptance of Near Infrared techniques in various fields has been discussed.

Keywords— ASTM, GMO, Kjeldah, NIR, transfectance.

I. INTRODUCTION

The recent development in instrumentation has supported the extensive penetration of Near Infra Red (NIR) Spectroscopy and imaging. NIR Spectroscopy is a fast and nondestructive analytical technique that provides chemical and physical information of any complex mixture. Using multivariate analysis, both quantitative and qualitative analysis could be done in no time. NIR spectroscopy has been gaining wide acceptance in varieties of applications like Food and Drug Industries, Petroleum, Pharmaceuticals, agriculture and many more.

II. MOTIVATION FOR FOOD GRAIN ANALYSIS

Food producing industries are always interested in quality assurance across the supply chain. Globalization and rising competitiveness forces producers to take strategic action for quality control and product optimization. Quality control and quality assurance are typically performed using classical chemical methods. Such methods usually take considerable time to produce results and involve utilization of harmful chemicals. Consequently, the results are not obtained quickly enough to meet the needs of Operations. Modern analysis techniques and software can provide an even better inside view into your raw materials and products within no time almost as if online.

Food composition databases provide detailed information on the concentrations of nutrients and nutritionally important components in foods. Calculating the nutrients facts from each its ingredient and its percentage is a need of food industry so crop yield would earn well for farmers as well as end users. The development of new and increasingly sophisticated techniques for the authentication of food products continues apace with increasing consumer awareness of food safety and authenticity issues. Food authentication is also of concern to

food processors that do not wish to be subjected to unfair competition from unscrupulous processors who would gain an economic advantage from the misrepresentation of the food they are selling.

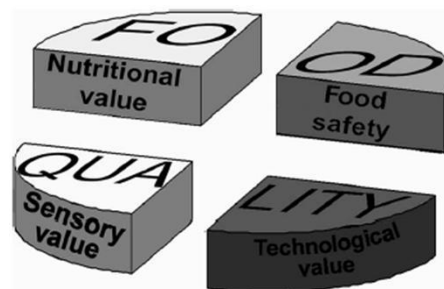


Fig.1. Factors influencing food quality

It is most important to also know the biological values of the food in terms of its sensory values like Genetically Modified Organism (**GMO**). The need of knowing the GMO values are felt and being researched in most agriculture universities. Considering all such aspect, various techniques for the analysis of food are gaining significance presently.

III. CONVENTIONAL TECHNIQUES OF FOOD ANALYSIS

The conventional techniques adopted for food content analysis like fat, protein etc. are standard chemical techniques developed and approved globally. Table-1 reflects standard tests adopted for some of the food constituents.

Table-1 : Recommended chemical tests for food

Parameter	Method	Reference
Protein	Kjeldah	Association of American Cereals and Chemists (AACC)
Parameter	Method	Reference
Oil	Single stage air oven	AACC

Moisture	Goldfisch Extraction	AACC
Crude fiber	Extraction	AACC

The important test for Protein which is approved is Kjeldah test which is comprised of three stages like Digestion, Distillation and Titration. The N-H bonds in protein by use of Sulphuric acid are broken and converted into ammonia (NH_3) and which in turn by means of a distillation process is separated from liquid phase. Titration is used to find the concentration of Protein in the sample. As the test itself is comprised of unit operation and process, it consumes time to deliver the results and a tedious process too. Hence in cases where online analysis is must, NIR is the only solution has been popularly accepted for food analysis.

IV. HISTORICAL BACKGROUND

Near Infrared radiation was discovered by Friedrich Wilhelm Herschel in 1800 (Davies, 2000) and covers by definition wavelength range from 780 to 2500 nm. When radiation hits a sample, the incident radiation may be reflected, absorbed or transmitted, and the relative contribution of each phenomenon depends on the chemical constitution and physical parameters of the sample.

Although *Herschel* discovered light in the Near Infrared (NIR) region as early as 1800, even spectroscopy of the first half of the last century ignored it in the belief that it lacked analytical interest. The Earliest application of NIR was reported in the 1950s, but it was not until the 1970s that the group headed by *Noriss* used it to analyze agricultural food samples. The development of equipment featuring improved electronic and optical components and the advent of computers capable of effectively processing the information contained in NIR spectra facilitated the expansion of this technique in an increasing number of fields [15].

The literature reflects the changes in the potential and the appreciation of NIR spectroscopy. Thus Wetzel in 1983 deemed it a "Sleeper among Spectroscopic Techniques" on account of high potential with scan use[14]. McLure in 1994 published a paper entitled "The giant is running strong" because of its increasing number of applications in different field. Davies in 1998, putting forward future possible advances and applications, aptly described its potential as taking it "from sleeping technique to the morning star of Spectroscopy"[7].

The interest in NIR spectroscopy lies in its advantages over alternative instrumental techniques. Thus it can record spectra for solids and liquid samples without any pretreatment, implement continuous methodologies, provide spectra quickly and predict physical and chemical parameters from a single spectrum. These attributes make it especially attractive for straightforward, speedy characterization of samples.

V. BASIC PRINCIPLE OF NIR SPECTROSCOPY

The American society of Testing and Materials **ASTM** defines the NIR region of Electromagnetic spectrum as the wavelength range of 780 to 2500 nm corresponding to the wave number range $12820\text{-}4000\text{ cm}^{-1}$. The most prominent absorption bands occurring in the NIR region are related to *overtone*s and combinations of fundamental vibrations of $-\text{CH}$, $-\text{NH}$, $-\text{OH}$ (and $-\text{SH}$) functional groups. Fig-2 shows the NIR spectrum and chemical composition response at effective wavelengths.

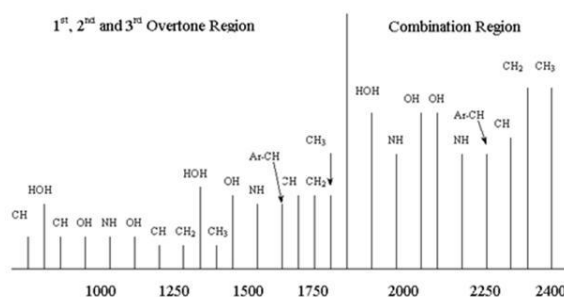


Fig-2 Constituent response at wavelength

The light in NIR band when irradiated on a sample under inspection, following three NIR absorbance phenomena take place.

Transmission

As has been clear from the Fig-3, the light in the NIR range falls from the source onto the sample and while passing through the sample, the sample depending on its constituents will absorb wavelength specific light which upon measurement from other side of the source will give result analysis. It is related to 1100 - 1800 nm wavelengths and used for high water content samples.

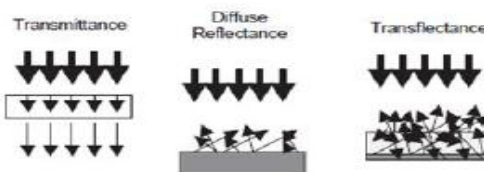


Fig-3 transmittance, reflectance and transflectance

Reflectance

In case of these phenomena, the light returned back due to the reflective properties of the sample would be measured for prediction of sample analysis. This phenomena covers 1800 - 2500 nm wavelength and used for earth samples and solids analysis.

Transflectance

A Transflectance phenomenon is the combination of Transmission and Reflectance as clear from the figure. Hence

reflected as well as transmitted light from the sample will be used for sample analysis predictions. Transflectance occurs in 800 - 1100 nm wavelength and used for slurries, grains and thick sample analysis.

VI. ADVANTAGES OF NIR SPECTROSCOPY

- ✓ It is a non-invasive, non-destructive technique.
- ✓ It requires minimal or no sample preparation. Solid samples can be directly measured with the little pretreatment, or no pretreatment, if an appropriate device is used.
- ✓ Measurement and result delivery are quite fast almost online. Dramatic developments in NIR equipment and chemo metrics used in conjunction with computers have enabled the real time extraction of analytical information from sample.
- ✓ There is no need for reagents or materials to prepare samples and the automation of technique results in increased throughput, which in turn, reduces analytical costs and decreases amortization time.
- ✓ A single spectrum allows several analytes to be determined simultaneously.
- ✓ The technique allows determination of Non-chemical (physical) parameters. In fact, the influence of some parameters on NIR spectrum allows the ready determination of properties such as density, viscosity pr particle size.
- ✓ Because of great strength of optical materials and robustness of NIR equipment, which in most cases has no moving parts, NIR instrumentation is most suitable for use in process control at production level.
 - ✓ Fiber optics provides robust, strong sensors for at-line, on-line and in-line analysis to control processes.
 - ✓ NIR spectroscopic results are comparable in accuracy to those of other analytical techniques, also, their precision is usually higher, because there is no need for sample treatment.

VII. DISADVANTAGES OF NIR SPECTROSCOPY

- ✓ NIR measurements are scarcely selective so chemometrics techniques have to be used to model data from which to extract relevant information.
- ✓ There are no accurate models to take account of the interaction between NIR light and matter. As a result, calibration is purely empirical in many cases.
- ✓ Accurate, robust calibration models are difficult to obtain as their construction entails using a large enough number of samples to encompass all variations in physical and/or chemical properties.

- ✓ The need to incorporate the physical and chemical variability of samples in calibration entails using as many as different calibration models as there are sample types, and hence more than one model per analyte.
- ✓ The technique is not very sensitive, so usually it can be applied only to major components.
- ✓ The NIR spectroscopy is a relative methodology, to construct models using it requires prior knowledge of the value for the target parameter, which must be previously, determined using a reference component.
- ✓ The construction of NIR models requires substantial investment, which can, however, be amortized by transferring calibrations from the master equipment to several slaves [15].

VIII. CURRENT TRENDS IN NIR RESEARCH

The use of near infrared spectroscopy has gained momentum and has been used to determine ripening time, probable crop yield time of vegetable/fruit etc. The biggest edge of NIR spectroscopy over conventional chemical techniques is the almost online result. Most research area of interest is the medicine and agriculture field. The publications recently published have increased significantly suggesting the approval of NIR spectroscopic analysis.

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