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Outlook of Near-Infrared Spectroscopy in Foodstuff Analysis

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Abstract- Near-infrared spectroscopy (NIRS) is a transformational tool in the analysis of food products. The two primary factors contributing to the success of the food sector are food quality and safety compliance. As a result, understanding the composition and utilizing technology to improve the food's quality, safety, and efficacy is essential. NIRS can significantly contribute to this. It may enhance the food industry by expediting the quality assessment of food. There are abundant references to the effectiveness of NIRS measurements combined with machine learning in determining food item quality, with auxiliary food item quality comprising constituents. This study aims to explain all the aspects of the research that have applied NIRS technology regarding food integrity analysis.

Keywords- Near-infrared spectroscopy, Quality control, Food safety, Chemometric techniques

I. INTRODUCTION

Food is the conglomeration of multiple components that can be labeled either nutrients or non-nutrients. Nutrients are usually categorized as macronutrients or micronutrients. Macronutrients (carbohydrates, proteins, and fats) are required in vast quantities to serve as foundations for cellular frameworks and substrates for energy in all living beings, whereas micronutrients (vitamins and minerals) are required in trace amounts for protein and enzyme activity [1]. There are deeply intimate links between humans and food. Most importantly, food security recognizes the cultural dimension of food security [2]. By 2050, the number of people worldwide is expected to reach 9.7 billion, presenting issues in accessing safe, nutritious, healthy food for all. To meet demand, food production must increase by over 50% of 2012 levels by 2050 [3]. In an ideal scenario, food is safe and conducive to good health, with the sole concern being the level of nutritional quality it possesses. However, complications arise when natural phenomena and human-related influences come into play, thereby giving rise to the issue

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of food safety, which encompasses matters such as freshness, microbial contamination, physical impairment, the presence of harmful substances, and instances of adulteration [4]. Today, food industries around the world face product quality and safety demands from consumers because of the growing need for health, quality, safety, and trust. Unsafe food consumption is having an adverse effect on both the health and social advancement of individuals. It is a difficult challenge for food manufacturers, processors, and operators to guarantee that the food they produce will not negatively impact consumers' health [5]. Hence, we need fast and non-disruptive methods that can be applied for assessing the quality of food products. Quality of food depends on its nutritional, physical properties, and flavors. Food that might be toxic, or food with poor nutrients, can all affect the quality of food, and perhaps even the health of the customer.

The development of quick and accurate diagnostic instruments has been further mandated to address the issue of food fraud, which is a big concern in the field of food safety [6,7]. Adulteration in postharvest processing has become more feasible due to the rising cost of produced food and agro-products and the ever-increasing population [8]. Pesticides and adulterants in food may cause a health risk. Pesticides can damage our human health, especially to the skin, digestive tract, and the respiratory system. Eating food contaminated by pesticides is one of the most common ways people come into contact with pesticides [9]. In a variety of scientific and analytical fields, traditional detection technologies, including “high performance liquid chromatography”, “ultra performance liquid chromatography”, “gas chromatography”, and “mass spectrometry” are generally used [10]. Although these processes are effective, they are known to be intrusive and non-real-time, involving time-consuming sample preparation and data processing [11]. In that light, the option of spectroscopy technology, encompassing near-infrared wavelengths, presents a potent solution to tackle several of the previously mentioned drawbacks, as it facilitates a non-invasive assessment that is swift, straightforward, environmentally friendly, and conducted directly on-site[12, 13].

The combination of Near-infrared spectroscopy (NIRS) with a machine learning based chemometric technique has been widely demonstrated to be an efficient food analysis technique. These techniques are essential for fully utilizing data and maximizing the knowledge gathered about processes, interactions, and features of the sample [14]. Chemometric technique extracting information about mutual relations between variables and reducing the multidimensionality of data. When multidimensional data is acquired through spectroscopic methods, chemometric methods appear to be highly beneficial [15]. Conventional approaches, particularly those that utilize "principal component analysis(PCA) and partial least squares (PLS)", have proven efficient in modeling near-infrared, or NIR, data when combined with spectroscopic methods of pre-processing based on experience. However, to improve model efficiency and effectiveness, deal with non-linearities in data, machine learning non-linear models are employed [16]. This approach has been extensively employed for qualitative analysis, product authentication, adulteration detection, and the differentiation of sample geographical origin, also to study molecules, aromatic, and biological compounds in food [17].

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II. DETECTION OF QUALITY PARAMETERS

I. *Moisture Content*

The amount of moisture present in a food is regarded as a critical factor in the assessment of food quality and is typically expressed as the proportion of water present in the food. The optimal moisture content for a food product will vary for various types of food products and their intended use. For example, low moisture content is desirable for food products that are going to be stored for a long time, such as dried fruits and vegetables. High moisture content is desirable for food products that are going to be eaten fresh, such as fruits and vegetables. To restrict microbial multiplication, it is necessary to keep the amount of moisture and water activity below approximately 10% and 0.60-0.65, respectively, based on the specific food category. Perishable food items, characterized by high moisture content, typically exhibit a water activity level nearing 0.99, rendering them highly susceptible to microbial propagation. Hence, an assessment of the moisture content in food items is essential to facilitate appropriate measures for preservation or alteration of the food product [18].NIRS detects harmonics and combination bands in molecular vibrations. Within organic molecules, common vibrations are observed in "functional groups" such as CH, -NH, -SH, and -OH, with the -OH component having an especially strong near-infrared absorber. This is also why the quantification of moisture is a fundamental application of NIR spectroscopy. NIR spectroscopy finds utility in determining water content in solids, liquids, and slurries. The moisture detection limit for solids is approximately 0.1%, whereas for liquids, it falls within the range of 0.02% (200 mg/L). Nevertheless, in specific instances, moisture detection limits as low as 40–50 mg/L have been attained [19].

The moisture content (MC) is a critical quality factor that is monitored and measured throughout the food industry& processing, and storage processes. Some commercial devices use measurements of near infrared radiation to measure the amount of moisture present in different types of products made from grains without requiring a sample for processing. However, the kernels of peanuts need to be broken up into smaller pieces and put into the “measuring cell” to use these devices to measure the MC of peanuts. This is harmful, takes a lot of time, and also comes with a lot of burden. Research has introduced an “NIR reflectance method” that enables the rapid and non-destructive determination of the average MC of approximately 100g of whole kernels.

The peanut grains that were tested had a MC range of 8%to 26%. Firstly, "partial least squares regression (PLSR)” was utilized to predict the results, and NIR reflectance observations were made at 1-nm gaps between 1000 and 1800 nm in wavelength. According to the conventional air-oven procedure, the numbers were compared to the predicted values of the samples analyzed in the aforementioned range. The readings from the "air oven" agreed closely with the ones that were anticipated, as evidenced by an R2 value of 0.96 and a standard error of prediction (SEP) of 0.83.

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II. *Protein*

Polymers of amino acids make up proteins. Proteins contain twenty distinct kinds' amino acids... Variation in proteins arises from the amino acid type, number, and sequence in the polypeptide backbone. This leads to differences in molecular structures, nutritional qualities, and physicochemical characteristics. Protein has an important function in cuisine because of its many advantages. They deliver vital amino acids, including "methionine", " tryptophan", and "lysine", as well as energy. Although the body is unable to manufacture certain amino acids, they are essential for human health. Furthermore, proteins are essential structural elements found in a variety of natural diets, influencing texture. Analysts study proteins in food to understand their concentration, type, structure, and functions."Brewer Johann Kjeldahl" developed the "Kjeldahl technique" in 1883.

Food is treated with a strong acid to release nitrogen, which is then measured through titration. The quantity of protein is determined by the percentage of nitrogen in the diet. Though several advancements have been made to expedite the procedure and acquire more precise measurements, the identical fundamental methodology is still applied today. The "Kjeldahl method" is commonly accepted as the method for determining the concentration of protein because it does not directly test the protein content. A conversion factor (F) is needed to translate the measured nitrogen concentration into a protein concentration. Each protein has a unique factor of conversion based on its amino acid composition [21]. The amino acids include groups like the amide group (-CON)and C-H bonds present in the side chains and backbone of amino acids in proteins that absorb light from the NIR region and are the key absorption bands relevant to proteins.

Rice is commonly acknowledged as a fundamental crop, serving as a substantial source of energy for individuals globally. The market value of rice is greatly impacted by its quality. Rice varieties with elevated protein levels tend to exhibit a firmer texture post-steaming, consequently influencing the overall flavor profile. The NIR spectra often display notable correlations and overlapping peaks, necessitating the utilization of "partial least squares regression (PLSR)" to manage spectral covariance. The integration of NIR spectroscopy with PLSR has garnered significant acceptance in the food sector, particularly for activities like estimating "Total flavonoid content" plus "phenols" in peanuts, evaluating reducing sugars in sweet potatoes, and. In quality of rice evaluation, "NIR spectra" are utilized to ascertain both amylose and amino acid concentrations in rice kernels. To assess various algorithms' modeling performance, PLS calibration models were created using Feature Wavelengths (FWs) chosen by "BiPLS", "BiPLS-GSA", and "BiPLS-SABPSO". Models were evaluated against "CARS", "Full-PLS"," BiPLS-GA", "BiPLS-SA", and "BiPLS-BPSO".

In terms of wavelength selection, "BiPLS-GA"," BiPLS-SA", and "BiPLS-BPSO" were in line with "BiPLS-GSA" and "BiPLS-SABPSO". Lowest "RMSECV" wavelengths were chosen as "FWs" after five runs of "CARS"." R2"," RMSE", "rRMSE", and "RPD" were used to assess the model's efficiency. Rice protein regression models using multiple "FW" methods of choice outperformed the full spectrum model with "R^2s" greater than 0.94, "RMSEs" less than 0.24%, "rRMSEs" less than 3.41%, and "RPDs" greater than 4.03, showing superiority to full spectrum models. The "BiPLS-SABPSO" model detects

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accurately than the “BiPLS-GSA” model, with R^2 of 0.949 and 0.956, rRMSE of 2.621% and 3.118%, and RPD of 4.235 and 4.500 for Vset and Tset, meeting rice protein content determination needs. The SABPSO algorithm was found to be more stable than “GSA”, and "SABPSO" and "BiPLS" were combined to create "BiPLS-SABPSO", which demonstrated effective FWs optimization efficiency. Therefore, it was determined that the NIRS combination and "BiPLS-SABPSO wavelength” and choosing fersanew is a novel concept for a quick, easy, and inexpensive model for detecting the quality of agri commodities. [22]. Intermolecular hydrogen bonds may enable them to be distinguished by their absorption intensity even though the sugar configurations are similar and exhibit similar NIR absorption peaks [23]. The primary vibration simplified encompasses the stretching and bending of these linkages. In a broad sense, Monosaccharides (glucose, fructose), Disaccharides (sucrose, lactose), and Polysaccharides (amylose, fructan) are able to be analyzed via NIRS [24]. Although they are still detectable, the absorption bands associated with the O-H and C-H groups in sugars—sucrose has eight O-H functional groups, while glucose and fructose each have five—have a major influence on the spectrum variations [23].

A prompt and accurate quantification technique was developed and authenticated for the simultaneous and non-destructive measurement of the sugar levels(Glucose, Fructose, and Sucrose)in intact apples by utilizing Fourier transform near-infrared(FT-NIR)spectroscopy in diffuse reflectance mode. Spectral pre-processing techniques, including mean centering, the second derivative of Savitsky-Golay, and multiplicative scatter correction (MSC), were used. Partial least squares (PLS) regression analysis was used to build the calibration models, and the high-performance liquid chromatography (HPLC) method was followed for method validation. To obtain the correlation coefficient of determination (r) and the least root-mean-square error of prediction (RMSEP), the spectral range and PLS factors number were optimized.

The most effective models exhibited reliable predictions, with RMSEP and r values for glucose being 0.201 and 0.950, for fructose 0.298 and 0.968, and for sucrose 0.335 and 0.969, respectively. The FT-NIR assessment of sugar levels in intact apples was observed to be more adaptable and efficient compared to the HPLC approach [25]. Amylose plays a crucial role in determining the nutritional value of rice. The quantity of amylase present impacts various characteristics, including the texture, retrogradation behavior, and viscoelasticity dynamics of rice starch gel.

Traditional methods for measuring amylase levels, like the iodine binding technique, face limitations due to species-specific iodine affinity and inconsistencies in reproducibility among different research institutions. Consequently, there is a demand for more accurate and effective analytical approaches, such as Near-Infrared (NIR) spectroscopy, which provides non-invasive analysis requiring minimal sample preparation. A study conducted by [26] utilized Near Infrared Spectroscopy (NIRS) to forecast the amylase concentration in 186 samples of yam flour. Partial least squares (PLS) and convolutional neural networks (CNN) were the two calibration techniques developed and tested on a different dataset. Metrics, including the coefficient of determination (R2), root mean square error (RMSE), and the ratio of performance to deviation (RPD), were calculated using predictions from an independent

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validation dataset in order to evaluate the final model performances.

The examined models exhibited varying performances (specifically, R2 of 0.72 and 0.89, RMSE of 1.33 and 0.81, RPD of 2.13 and 3.49, respectively, for the PLS and CNN models). In accordance with the standards of quality for NIRS model prediction in the realm of food science, the PLS approach was deemed unsuccessful (RPD3 and R20.8) in the prediction of amylase content in yam flour, whereas the CNN model was validated as a dependable and effective methodology. This study demonstrated the feasibility of utilizing NIRS as a high-throughput phenol typing method to accurately predict amylase content, a critical factor in the quality and acceptability of yams, through the implementation of deep learning techniques.

III. Fats

Triglycerides, or fats, are lipids that consist of three fatty acid molecules and glycerol. Long hydrocarbon chains with a carboxyl group (-COOH) at one end are known as fatty acids. The chemical structures of dietary fats can be used to differentiate between saturated and unsaturated fats. At ambient temperature, saturated fats are solid due to the complete bonding of carbon atoms with hydrogen. These fats, which are composed mainly of saturated fatty acids, can be found in red meat, poultry, whole-milk dairy, butter, eggs, and specific oils, which have the potential to elevate LDL cholesterol and increase the risk of chronic heart disease if eaten in excess with no physical exercise.

Oils are lipids that are liquid at room temperature. They are typically derived from plants and fish. Common examples include olive oil, canola oil, and fish oil. Oils are rich in unsaturated fatty acids. This category includes both monounsaturated and polyunsaturated fats, which are considered beneficial for heart health [27]. Fatty acids; carbon-hydrogen (C-H) bonds are the most significant factors in the NIR absorption spectra. In the near-infrared region, these bonds show overtone and combination bands. Specifically, the second and third harmonics of the C- H stretching vibrations (approximately 1700-1800 nm and 2100-2300 nm, respectively) are conspicuous in NIR spectra and are employed to quantify fat content. The absorption of NIR is also substantially influenced by the methylene (CH2) and methyl (CH3) groups in fatty acids and triglycerides. The characteristic absorption bands that these groups produce are correlated with fat content due to the symmetric and asymmetric stretching and bending vibrations [28]. A study on hamburgers suggested a substitute analytical method for determining the fat level of industrial chicken, which is based on the Successive Projections Algorithm for Interval Selection in Partial Least Squares Regression (iSPA-PLS) and Near Infrared Spectroscopy (NIR).

In order to achieve this, 70 chicken hamburger samples were prepared with a fat content ranging from 14.27 to 32.12 mg kg^{-1}, in accordance with the Argentinean Food Codex maximum limit of 20% (w/w). After that, the NIR spectra were obtained. The intense spectral bands at 5150 cm^{-1} (a result of O-H stretch and deformation) are mainly responsible for the water. The first overtone of the O-H stretch vibration is 6900 cm−1. As an amide, the protein is associated with the absorption band at 5900 cm^{-1}. Other peaks at 8350cm−1 (the second overtone of-CH stretch), 5800–5700cm−1 (the first overtone of-CH stretch), and 4300–4260cm−1 (combined stretch and deformation band) correspond to fat content. The data were preprocessed using a variety of methods, including baseline correction, SNV, MSC, and Savitzky-Golay smoothing.

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Additionally, the Interval PLS and full-spectrum PLS are implemented for comparison. With a window size of 19 points and a second-order polynomial, the first derivative Savitzky-Golay smoothing obtained the best results for the prediction set, with an RPD of 3.02, an RSP of 7.69%, an RMSEP of 1.59 mg kg-1, and a correlation coefficient of 0.94. Because it doesn't produce pollution and doesn't call for the use of chemical reagents or solvents, the suggested methodology is a better option than the conventional Soxhlet extraction method and is consistent with the core ideas of green chemistry. At a 95% confidence level, the results of the analysis of chicken hamburgers using the novel method agreed with the reference values. As such, it is very attractive for regular analysis. [29].

IV. CONCLUSION

The utilization of Near-Infrared (NIR) spectroscopy in food quality analysis has exhibited exceptional potential, offering a non-destructive, eco-friendly, and efficient approach to the monitoring of a variety of food components. The utilization of sophisticated machine learning algorithms, including neural networks, in conjunction with NIR spectroscopy has substantially improved the reliability and accuracy of food quality assessments. It has been demonstrated in research that NIR spectroscopy is capable of accurately detecting adulterants, predicting the talc content in wheat flour, and determining the moisture content in food products. In spite of its numerous benefits, there are still obstacles, including the necessity for user-friendly data processing solutions and robust calibration models. These obstacles are anticipated to be surmounted by advancements in data fusion and deep learning technologies, which will facilitate the implementation of NIR spectroscopy in the food industry on a more widespread scale. In conclusion, one promising method for guaranteeing the quality and safety of food is NIR spectroscopy, which is in line with the increasing demand for rapid and dependable food analysis techniques.

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