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# Application of Spectral Analysis Technology in Food Safety and Quality

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***Abstract:*** *With the development of science and technology, food detection technology has been improved. The rapid, high efficiency, high accuracy and non-destructive of spectral analysis technology overcome the defects of traditional food detection technology to a certain extent, and has been widely used in the food detection industry. In this paper, the concept, classification and application of spectral analysis technology are introduced through three topics, especially two common spectral analysis technologies; The application of the technology in food detection industry is illustrated by examples, which shows the advanced and superiority of the spectral analysis technology, and lays a foundation for the popularization of the technology.*

***Keywords:*** *Spectral analysis technology; Food safety and quality; Application; Overview*

## 1. Introduction

Traditional means of food quality inspection not only have to be carried out in specialised laboratories, which require experimental space and equipment, but also consume a great deal of human and material resources, while placing certain requirements and limitations on the professional skills of the testing workers, and the samples being tested need to be pre-treated in advance, which greatly increases the risk of sample damage [1]. Compared to other traditional analytical instruments, spectroscopy is regarded as a new, non-contact method of detection and is therefore favoured by researchers. The spectroscopic detection technique allows for fast, efficient and highly accurate detection without compromising the quality of the sample. The method is simple to operate and does not require a high level of skill from the testers and staff. Spectroscopic analysis techniques can comprehensively and rapidly resolve information on the chemical structure of sample molecules, the concentration of substances and the interactions between molecules, and are therefore very widely used in industries such as food safety testing, pharmaceuticals, chemicals, materials and the environment [1]. However, spectroscopic techniques are not yet widely used due to their expensive instrumentation and cumbersome data processing [2].

### *1.1 The Overview of spectral analysis technology*

Spectral analysis technology is an important instrument analysis method for food detection according to the absorption of substances or radiation radiated energy, because the atomic groups of different chemical molecules and the spectrum of chemical elements emission and absorption are different, and the same chemical composition under some special conditions, the spectral intensity of its emission and absorption is proportional to the content of these chemicals, so we can use this feature to conduct qualitative and steady-state quantitative analysis of various substances, such technology is called spectral analysis technology.

This technique is favored by many experts in food safety and quality inspection, such as Table 1 to analyze the composition or content of certain substances. Generally, the detected substance has a basement state electron, but under electromagnetic wave irradiation, the electron absorbs a certain wavelength of light energy into an excited state, and the electrons in the substance emit different forms of energy, which mainly refers to the electric or magnetic field that oscillates in phase and is perpendicular to each other [1]. When a beam of light comes into contact with other substances, it will absorb or emit electromagnetic radiation in the form of quantum, thereby transferring the quantum

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structure of the material and the energy levels between them, and spectral analysis is achieved by using this transfer of energy levels between the two sides. Different electromagnetic waves have their propagation distance (wavelength) λ during the vibration period or the number of periodic changes υ (frequency) per unit time. In a space where the pressure is lower than atmospheric pressure, the relationship between wavelength λ and frequency υ is c = λυ, frequency has nothing to do with the medium, and different media will only have an effect on the wavelength of light. We can use the principles of spectral analysis technology to inspect and analyze food. For example, spectroscopic analysis techniques can accurately determine the content of food additives in food parts. At present, in China's food safety quality testing, the application of spectral analysis and detection technology has obvious technical advantages, such as the use of spectral technology to facilitate the operation of inspectors, small damage to samples, high inspection efficiency [3-6] and other advantages. Spectral analysis technology has a very strong ability to identify and distinguish different elements, and they can also detect mixtures of multiple elements with very high accuracy. Spectroscopic technology can not only realize the protection of the environment, but also realize the effective monitoring of the environment, and the environmental impact is small, which is a new technology with great development prospects. When testing the sample, light and the substance act on the sample, do not need to contact the sample to be tested, reduce the damage to the sample, and have the advantages of low cost and fast detection; At the same time, with the continuous development and upgrading of spectral detection instruments and chemometric methods, the detection accuracy has gradually improved, which has led to the wide application of spectral detection technology in the field of food safety and medicine. Common food safety detection spectroscopy methods include: near-infrared spectroscopy, Raman spectroscopy, etc.

*Table 1: Spectral Analysis Technology In Food Safety And Quality*

| References | Detection method | Detect targets | Analysis method |
|---|---|---|---|
| Tito et al.(2012)[7] | Near-infrared spectroscopy | Total oxygen demand | Principal component analysis, PLS modeling |
| Masounm et al.(2012)[8] | Near-infrared spectroscopy | Crude protein | PLS modeling |
| Olsen et al.(2008)[9] | Ultraviolet and visible spectroscopy /Near-infrared spectroscopy | fat content | SW-MLR modeling |
| Huang et al.(2001)[10] | Near-infrared spectroscopy | Salt content | BPNN modeling |
| Wold et al.(2004)[11] | Raman spectroscopy | Carotenoid content | PLS modeling |
| Elmasry et al.(2008)[12] | Near-infrared spectroscopy | fat content | PLS modeling |
| Zhu et al.(2012)[13] | Ultraviolet and visible spectroscopy | sugar content | LS-SVW modeling |

## 2. Application of Near-infrared spectroscopy in Food Detection

The reason why near-infrared spectroscopy (NIRS) has become a fast and efficient powerful tool for online online analysis is determined by its technical characteristics, the main technical characteristics of NIRS are as follows: (1) Fast analysis and detection speed. Since the chemical detection and correction of a single optical spectrum is usually less than 1min, the computer analysis model established and corrected by itself can quickly and accurately determine and derive the chemical composition of the spectral sample or the physical properties of the chemicals used; (2) High analysis efficiency; (3) Low cost of use; (4) Good test reproducibility; (5) No pre-treatment required; (6) Facilitate online analysis; (7) Non-destructive analysis.

### *2.1 Application in fruits and vegetables*

NIRS glucose detection technology, mainly used in the monitoring and inspection of fruit and vegetable product quality, the main fruit and vegetable varieties that can be applied are citrus, watermelon, dragon fruit, tomato, etc., as well as cabbage, olives, kale, etc. At present, the main content of testing is the detection of glucose, vitamins, total acid and hardness, and the quality and stability control of fruits and vegetables during storage. Yuan Lei et al. [14] used NIRS to establish models of partial least squares regression (PLS) detection of various common nutrients in citrus. Li Guifeng et al. [15] constructed a multiple linear scattering function and correction (MSC) method for detecting the quality and hardness of various apples, as well as a multivariate scattering correction and partial least squares regression (PLS-

MSC) expectation model for the hardness of various apples, R (indicating the quality of the linear regression model, the larger R, the closer the value predicted by linear regression is to the true value; It also indicates that the linear correlation coefficient between the observed value and the model description value, the larger the better) is 0.9652.

In the supervision and sampling inspection and management of the safety and quality of fruit and vegetable products, the main testing contents involved generally include: the detection of microorganisms or harmful substances, the traceability of the place of origin, whether adulterated, etc. Zhou Xiangyang et al. [16] et al. used the NIRS digital model to investigate the effect of practical application, took the commonly eaten vegetable varieties as the detection object, and analyzed it by gas chromatography-mass spectrometry (GC-MS), as a verification and other research methods, the residues of various phosphoric acid chemicals and agrochemicals in the plants and leaves of more than 20 crops such as Peony and Chrysanthemum were comprehensively analyzed, and many satisfactory results were achieved. Ma Benxue and other experts [17] through in-depth study of NIRS analysis and detection technology, established the corresponding judgment standard methods for peeling calyx fruit, and proposed to establish a spectral database and stability of different populations and classes of Fragrant cecalyx of the Korla subfamily Pear/Cebu calyx fruit, and the judgment accuracy of the correction set and detection set was basically 100% and 95%, respectively. Xie Lijuan et al. [18] used MSC data statistical analysis to classify natural genetic engineering crops and non-natural genetically engineered crops, such as tomatoes and other food categories, and the identification accuracy rate could directly reach 89.7% on average.

### *2.2 Application in meat products and aquatic products*

At present, NIRS focuses on the safety detection and analysis of meat products, focusing on the comprehensive assessment of safety quality and safety management performance of four meat raw materials, pig, cattle, sheep and shrimp. Wang Xichang et al. [19] detected the water and protein content of two surimi by NIRS and the water content correction model established by PLS method at the same time, and the R values should be 0.98 and 0.96, respectively. Sun Shumin et al. [20] were able to accurately distinguish and judge sheep from five different origins through NIRS analysis combined with principal component analysis (PCA) linear analysis, with an analysis accuracy rate of 91.2%. In terms of egg component analysis and safety detection, Wu Jianhu et al. [21] et al. used NIRS and spectral analysis detection technology to accurately detect and correct the protein content in fresh ready-to-eat egg liquid, and the corrected test result R was 0.89. Giunchi et al. [22] comprehensively use the functions PCA, PLS and other methods to carry out nutritional modeling and analysis of various raw egg agricultural products, detect their freshness, and classify and detect according to the storage and shelf life specified by the location of the product, and the accuracy can generally reach 100% directly.

### *2.3 Application in detection of dairy products and beverages*

The new generation of technology using NIRS combined with optical fiber networks can realize the networked detection of the content of all biological macromolecules in different types of dairy milk in different captive areas. Wang Caiyun et al. [23] analyzed and detected the toxic residues such as spectinomycin, gentamicin, neomycin, streptomycin and their content changes in China's milk powder by using NIRS and PLS, and the R reached 0.9893. Wang Youjun et al. [24] used NIRS to determine milk mixed with mineral salts and natural plant proteins, respectively, and the R was 0.969 for products with a large amount of organophospholipid hydrolysate and phospholipid protein powder. Yuan Shilin et al. [25] used PLS combined with least squares vector machine (LS-SVM) technology to reconstruct a model that can detect melamine content in high-quality milk powder, and R can reach 0.9109. Wang Yunli et al. [26] detected the concentration and content of four phthalates in a black tea beverage by using the mathematical model established by PLS, and R should be 0.9895, 0.9927, 0.9842 and 0.9879, respectively. Chen Meili et al. [27] scholars used NIRS and infrared spectroscopy interaction combined with stoichiometry and statistical physics to analyze and detect the chemical composition data of thirteen tea leaves, including tea polyphenols, theophylline, steeping products, gallic acid and sugars, and all R values reached more than 0.7, with high accuracy.

### *2.4 Applications in wine, edible oil and condiment testing*

The application of NIRS in wine production and brewing mainly focuses on the rapid detection and analysis of various component parameters and metal elements in wine, and also uses NIRS to synchronize the detection and research of various parameter changes in the process of wine fermentation. Chen Yan et al. [28] established a corresponding calibration model by using the PLS method to determine the content of key indicators such as ethanol, total acid, total ester and ethyl caproate in liquor, and the R value was about 0.67~0.97. Yuhui et al. [29] used PLS method to achieve rapid non-destructive detection of methanol exceeding the standard, and the R value reached 0.9998. The test products of Liu Wei et al. [30] are based on the Fisher discrimination model, and the accuracy rate of Fisher discrimination of wine origin can reach more than 86.7%.

NIRS is mainly used in the basic rapid monitoring and quantitative analysis of edible oil quality, and the main content can be roughly divided into two categories, one is the analysis of key quality parameters, including the analysis of edible oil quality, as well as the traceability of its origin source, whether it is gutter oil, etc.; The other category mainly refers to rapid quantitative analysis and detection, which mainly includes rapid analysis and detection of the composition of the main components in various edible oil products, whether they are adulterated and the content of chemicals adulterated with counterfeit products. Chen Yongming et al. [31] proposed through research that NIRS based on information global search algorithm-genetic algorithm was used to analyze and model the situation of each olive oil producing area in China, and its traceability analysis could be up to 100%. Xue Yalin et al. [32] constructed a judgment model for the stability of vegetable oil through NIRS research, which can be applied to the rapid test of vegetable oil adulteration with high accuracy. Zhang Hui and other experts [33] used PLS analysis to detect the concentration of essential fatty acids in edible oil, and R has reached 0.989. Zhao et al. [34] simultaneously determined the content of amino acid nitrogen and total acid in soy sauce by near-infrared spectroscopy combined with characteristic variable selection method, and used PLS to determine and analyze all individual amino acids containing amino and carboxyl groups and the total value of all amino and carboxyl amino acids in soy sauce, respectively, and also jointly modeled them, where R can reach 0.9988 and 0.9902, respectively. Tu Zhenhua et al. [35] used PLS and other methods to identify honey adulteration based on NIRS, and accurately detected and identified the adulteration of the main components of various finished honey and the overall quality and performance characteristics of the product, and the accuracy rate of adulteration identification can generally reach 100%. Zhong Yanping et al. [36] used PCA method combined with NIRS to establish honey varieties and qualitative identification models of authenticity in different spectral regions, which can accurately identify and judge wattle honey, locust flower nectar, rape honey and adulterated honey, and the success rate of type judgment and authenticity identification can be as high as 90%. Han Donghai et al. [37] used PLS analysis combined with NIRS to construct a data model to detect the hardness of curd billet, where R was 0.935.

### *2.5 Application in the detection of rice, flour and their products*

NIRS is widely used in the field of safety testing of grain and oil raw materials such as corn, flour and rice, including the analysis of its main components and the testing of safety performance. Sun Xiaorong et al. [38] established a model using PLS method in NIRS through experimental research to identify flour mixed with talcum powder and other powders, where R was 0.994. Sun Jun et al. [39] et al. used PCA and support vector machine model (SVM) determination methods combined with NIRS and hyperspectral to comprehensively detect the adulteration degree of various refined rice, and the accuracy of detection can reach more than 90%. Ma Xuying et al. [40] used PLS modeling combined with NIRS to detect and analyze the dietary fiber content in oat and buckwheat samples, and the R was 0.9272.

### *2.6 Application in health food testing*

Tian Guohe [41] et al. used NIRS to illegally add metformin hydrochloride ($C_4H_{11}N_5$) to drugs used in traditional Chinese diabetic medicine and health foods, and the accuracy rate reached 98%. An Xuesong et al. [42] use near-infrared spectroscopy to analyze the content of trans fatty acids (TFA) in food with an accuracy of 88%. Shen Fei et al. [43] directly applied NIRS to the detection and analysis of octathion pesticide residues, used silica gel or silicate gel ($mSiO_2 \cdot nH_2O$) as an adsorbent to treat the samples, and established a data model with PLS for analysis, with an accuracy of about 90%.

## 3. Application of Raman Spectroscopy in Food Detection

Raman spectroscopy is often used to determine protein solubility, surface viscosity, water retention, surface texture characteristics, peroxide content, and fatty acid content in meat products [1]. The results show that Raman spectroscopy, as a new detection technology, has good consistency with the data obtained by conventional traditional detection techniques, indicating that there is a high correlation between Raman spectroscopy and the structure and chemical composition of the corresponding substances. Raman spectroscopy can clearly observe the changes in chemical components such as proteins and fats in meat products, and the information obtained from them can determine the type of meat products. In addition, Raman spectroscopy, as a new detection method, has unique technical advantages, it has low requirements for sample pretreatment process, simple operation, small pollution damage to the sample, and small number of samples required [44].

Due to the interference of both the animal's pre-mortem and post-mortem conditions, the quality of foods of animal origin can change drastically, unless they are handled with particularly rigorous and complex procedures. During the storage period of food, the overall nutritional value will continue to decrease, and various spoilage will occur, and the safety and quality of the product can be controlled and detected by observing the structural changes of muscle fibroprotein. Traditional chemical, physical and biological detection methods, such as solubility detection, surface viscosity, extraction rate, water storage capacity, etc., are not only time-consuming and laborious, but also have serious damage to the tested sample, and also cannot achieve portable detection and online monitoring on the network. Therefore, Raman spectroscopy detection has the advantages of robustness, rapidity and non-destructive compared with traditional product detection methods. Raman spectroscopy has the above advantages compared with traditional detection methods, and this technology has been successfully used in many fields for network online monitoring[45].

### *3.1 Application in dairy product testing*

There are three main methods and techniques for the detection of melamine chromatography, namely: high performance liquid chromatography, liquid chromatography-mass spectrometry/mass spectrometry, gas chromatography-mass spectrometry, and the detection limits of the detected substance should be 2, 0.05, 0.01mg/kg respectively[46]. Zhao Yuxiang et al.[45] studied the Raman spectral characteristic peak and its intensity at 708~714 cm-1 of melamine to detect it qualitatively and quantitatively. Under normal circumstances, common substances such as urea and nitrite have an impact on Raman spectroscopy, a rapid measurement method, so there is no interference, and each sample only takes an average of 10 minutes from sample preparation to test result, which greatly shortens the detection time. Chen Anyu et al. [47] used surface-enhanced Raman Scattering (SERS) detection technology to accurately identify the presence of melamine in cow's milk, defined the characteristic peak of melamine at 710cm-1 intensity, and corrected the numerical relationship between it and dimethylcyanamide, and finally detected a limit concentration of 0.5mg/kg.

### *3.2 Application in the detection of pesticide residues in grains and fruits*

Raman spectroscopy detection and analysis technology has been widely used in the determination and analysis of pesticide residues in grain, oil and fruits and vegetables, such as the detection of harmful chemicals and pesticides caused by the processing and use of various grains, fruits and vegetables; Other harmful chemical pesticides and residues of harmful chemicals after oxidation are quantitatively analyzed and detected, and certain technical research results and application progress have been made. Zhou Xiaofang et al.[48] et al. used a near-infrared Fourier transform Raman spectroscopy (FT-Raman) instrument with an excitation wavelength of 1064nm to conduct Raman tests on common fruits and commonly used pesticides, and obtained the characteristic Raman spectra of corresponding fruits and pesticides, and found that FT-Raman could well identify whether there were pesticide residues by the determination of three different types of insecticides (24.5% Ifodin emulsion, insect mite emulsion and Baoguonin No. 2 powder) common in the market. And good results have been achieved.

### *3.3 Application in the detection of food additives*

Malachite green is a synthetic triphenylmethane basic dyes, the main component is triphenylmethane, malachite green is easy to be absorbed by the fish body, forming colorless malachite green in the fish body, it is difficult to identify with the naked eye, the maximum limit of China's aquatic products is 0.5μg/kg, and the state prohibits the addition in the field of pollution-free aquaculture. At present, there are many methods for detecting malachite green, in the national standard, there are mainly the following methods, the detection limits are 2.0 μg/kg, 0.5 μg/kg, the use of Raman spectroscopy for the rapid inspection of malachite green, with good reproducibility, simple sample pretreatment, short detection time, low detection cost, simple equipment operation, and detection limit up to 5.0 μg/L, Gu Zhenhua et al. [49] used malachite green at 432~437$cm^{-1}$, The Raman spectral characteristic peaks and other

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characteristics of 1166~1170cm$^{-1}$, 1613~1617cm$^{-1}$ are quantitatively and qualitatively detected malachite green, and the detection limit is 0.5μg/L, and the whole detection process only takes 3min.

Sudan red is an industrial dye, not a food additive, and is carcinogenic. At present, there are three main detection methods for Sudan red, namely: liquid chromatography, thin layer chromatography and liquid chromatography-mass chromatography. At present, Raman spectroscopy has also been widely used in Sudan red detection. Sudan red I., II., III. has been detected by Raman spectroscopy, and its Raman spectrum has corresponding characteristic Raman peaks, so Raman spectroscopy can be widely used in the detection of Sudan red in peppers and other foods [50].

## 4. Summary

Compared with other traditional conventional chemical testing technologies, spectral analysis technology provides consumers with a safe, non-destructive, non-contact detection method, which can easily complete the chemical performance evaluation and certification of various products. This is mainly because thanks to the currently used spectroscopic technology, it is a network online detection, and does not have to spend a lot of time, and the operation is simple, no need to train and commission special personnel to operate, which greatly reduces costs, and is less affected by the external environment, reducing human error. Spectral detection is an ideal detection method to obtain the most data with the fewest samples without the need for complex sample preparation.

However, there are still some shortcomings in the experimental methods and related techniques for spectral detection analysis, such as the use of NIRS to accurately detect the concentration of various chemicals, in order to ensure that accurate spectral experimental data can be obtained quickly, in the initial stage of the experiment, a large number of known samples need to be used as a training set and modeled. The accuracy of NIRS assay data is largely determined by the reference value of the training set and the accuracy of the concentration of the prepared standard sample [1]. At the same time, NIRS may also have the problem of not accurately judging the physical and chemical information of the material corresponding to the infrared absorption peak, because NIRS is the frequency doubling and frequency combination region of the fundamental frequency of molecular vibration, so the spectral curve detected by NIRS contains a lot of complex information of other substances. As far as Raman spectroscopy is concerned, the biggest problem is that the detection equipment and instruments of Raman spectroscopy are too expensive compared with traditional conventional detection instruments, which limits the application of Raman spectroscopy detection technology in food quality and safety. In order to improve its signal intensity, short-wave laser light sources are usually used to solve this problem, but short-wave laser light sources are likely to cause fluorescence effects in the test sample, thereby masking the Raman signal, and too high laser energy will also have a certain impact on the accuracy of detection.

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