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A Review of the Applications of Spectroscopy for the Detection of Microbial Contaminations and Defects in Agro Foods

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Abstract

Recently, spectroscopy has emerged as a potential tool for quality evaluation of numerous food and agricultural products because it provides information regarding both spectral distribution and image features of the sample (i.e., hyperspectral imaging). Spectroscopic techniques reveal hidden information regarding the sample and do so in a non-destructive manner. This review describes the various approaches of spectroscopic modalities, especially hyperspectroscopy and vibrational spectroscopies (i.e., Raman spectroscopy and Fourier transform near infrared spectroscopy) combined with chemometrics for the non-destructive assessment of contaminations and defects in agro-food products.

Keywords: Agro-food, Chemometrics, Hyperspectroscopy, Microbial contamination, Vibrational spectroscopies

Introduction

Consumers consistently prefer superior quality food products, while defective or contaminated products are rejected owing to their potential for adverse effects on health. Therefore, quality and safety have become the primary factors that influence a consumer's choice in food products. Hidden defects or contamination are difficult to recognize with visual selection procedures, but intake of contaminated food causes food-borne illness; hence, identification of food contaminants is an important issue for ensuring food safety. Furthermore, contaminants will have a negative impact on the quality of food and agricultural products, thereby affecting the producing country's economy. Conventional methods such as high performance liquid chromatography (HPLC), immunoaffinity chromatography, and enzyme-linked immunosorbent assays (ELISA) are widely used for quantitative measurement of contaminants in food and agricultural products. The advantages of these methods are that they are sensitive, quantitative, and reliable, while the drawbacks are that these approaches are expensive, time consuming, labor-intensive, and require sample destruction (Gowen et al., 2007). Consequently, rapid and non-destructive measurement techniques are increasingly being used for quality control and for food safety.

Spectroscopic methods are successful, novel, and accurate for evaluating contamination and defects in agricultural and food products. These methods require minimal sample preparation and provide non-destructive measurements and have recently been incorporated into food quality and safety analyses (Huang et al., 2013; Sing et al., 2009; Wang, J. 2011). The main objective of this review is to evaluate the potential of various kinds of spectral modalities such as hyperspectroscopy and vibrational spectroscopies (i.e., Fourier transform near-infrared spectroscopy [FT-NIR] and Raman spectroscopy) that are used in the detection of contamination in food.

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Principles of the Spectroscopic Methods

Hyper spectral imaging (HSI) technique

The image generated by HSI is composed of numerous pixels of information (also called "spatial information") and spectral information of the sample, and the resulting image achieved through the HSI system is three dimensional (also known as a hypercube), holding two spatial dimensions and one spectral dimension (Figure 1). Thus, each image in the "hypercube" represents the chemical and physical features of the object (Wu and Sun, 2013, Hung et al., 2014). In addition, HSI is a non-destructive, rapid technique that enables contactless measurement of the samples (Kim et al., 2001).

In recent years, the HSI technique has been operated either in the reflectance or transmittance modes (Ariana and lu, 2008) in the range of visible and NIR (400-2500 nm) for quality classifications or predictions of food and agricultural products (Zhang, 2012; Kim et al., 2002; Cho et al., 2013; Wei et al., 2013). HSI is an emerging tool for detection of microbial spoilage (Ellis, 2002), fecal contamination (Chao, 2008) and skin tumors (Kim, 2010) in meat products. In fruits (Xing et al., 2005) and vegetables (Ariana et al., 2006), this technique is well suited for detecting contamination, bruises, and chilling injury (Mehl et al., 2004; Gowen et. al., 2009). In addition, HSI has great potential for detecting fungal contamination (Williams et al., 2012), toxic metabolites (Yao et al., 2013), and other forms of damage in grains (Bauriegel et al., 2011).

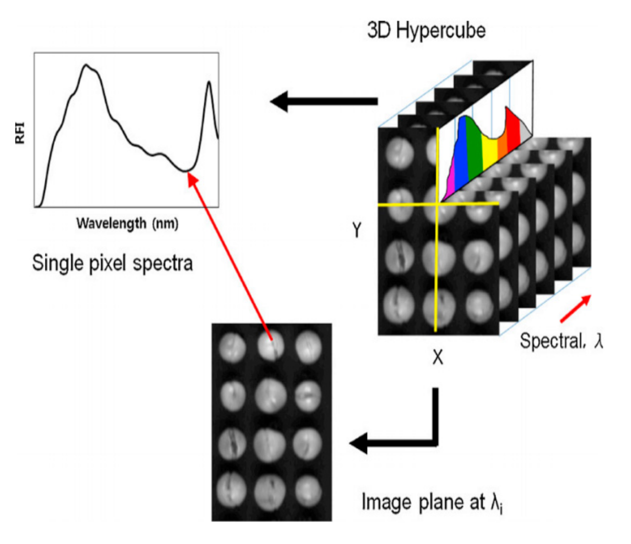

Figure 1. Schematic of a hyperspectral image structure; spatial axes x and y and spectral axis λ (Cho et al., 2013).

Vibrational spectroscopies

Fourier transform infrared spectroscopy (FT-IR)

In addition to the HSI technique, IR spectroscopy plays an important role in both industrial and research fields for evaluating food quality (Wang and Paliwal, 2007). IR radiation was first discovered by F.W. Herschel in 1800. IR spectroscopy is a non-destructive, reagent-free, and non-invasive technique based on the vibrations of specific chemical functional groups, particularly C-H, O-H, N-H, or C=O groups (Burgula et al., 2007). It is classified into near-infrared (NIR, 780 nm-3 μm), mid-infrared (MIR; 3-50 μm), and far-infrared (FIR; 50-1000 μm). MIR provides knowledge about the fundamental vibrations of sample molecules (i.e., their chemical structures) that are excited by the infrared beam, and the absorbance spectra in the MIR region represent the "metabolic fingerprint," characteristic of the sample. Since FT-IR spectroscopy provides faster and higher resolution spectra, it has been widely used for the detection of adulteration (Woodcock et al., 2008) and for authentication (Reid et al., 2006) of food products and for the analysis of sugars (Duarte et al., 2002) and acids (Beullens et al., 2005) in fruit and fruit juices. Additionally, FT-IR is often applied for simultaneous identification and quantification of bacteria and fungi in foods (Yang et al., 2003) like juices, meat, and grains (Al-Qadiri et al., 2006; Ammor et al., 2009).

Raman spectroscopy

Similar to IR spectroscopy, Raman spectroscopy is a technique used to measure the vibrational and rotational spectra of sample molecules. For measurement of Raman spectra, the substance is illuminated with a beam of monochromatic light from a laser source, and the scattered light from the sample is measured. The phenomenon of light scattering was first observed by Raman and Krishnan in 1928 (Smith and Dent, 2005). Raman spectroscopy provides better information about the symmetrical vibrations of the covalent bonds e.g., C=C and S-S than the IR spectroscopy (Lee et al., 2013). IR spectroscopy exhibits high interference from the water band, while Raman spectroscopy is relatively less affected by the water content, which makes it advantageous over IR spectroscopy and more suitable for the analysis of complex heterogeneous materials (Thygesen et al., 2003). In addition, compared to IR spectroscopy, Raman spectroscopy requires less sample preparation. Raman spectroscopy is more applicable to the determination of grain quality than is IR spectroscopy, because it has higher spectral resolution and distinct features (Lee et al., 2013).

Chemometric Methods

Since spectroscopic data are composed of enormous amounts of meaningless information, chemometrics methods are widely used to reduce high-dimensional data and retain essential spectral information that is further used for sample classification for food quality and safety purposes (Amigo et al., 2013). A couple of studies have used qualitative analysis based on principle component analysis (PCA), linear discriminant analysis (LDA), and k-means clustering for data dimension reduction, optimum waveband selection, and classification (Amigo et al., 2013). Artificial neural network (ANN) and multi-linear regression (MLR) techniques are also extensively used to obtain quantitative prediction or classification of sample features (Ammor et al., 2009; Li et al., 2011). Table 1 shows some applications of chemometrics in the evaluation of various foodstuffs.

Applications

Detection of microbial spoilage and fecal contamination in meat

Meat is a preferred food worldwide owing to its high nutrient content, which includes proteins and essential amino acids, (Feng et al., 2013) and because it is a rich source of vitamin B; therefore, global meat consumption has been steadily increasing over the last few decades. The continual demand by consumers for superior quality of meat necessitates the development of accurate and innovative detection techniques to comply with food safety and quality parameters. Improper refrigeration and processing methods lead to undesirable growth of microbes, especially of *Salmonella*, *Escherichia coli*, and *Campylobacter* pathogens, and psychotropic bacteria. These organisms can grow at low temperatures and cause spoilage of meat (Borch, 1996; Laursen, 2008). In addition, contaminated products are off-flavored and associated with health risks in humans (Feng and Sun, 2013). The application of conventional microbiological methods for the detection of microbial spoilage in meat, such as plating (Jongenburger et al., 2010), adenosine triphosphate (ATP) and (Champiat, 2001) and nucleic acid-based methods (Scheu, 1998), is limited, largely because they are very costly, time-consuming, and labor-intensive.

Recently, various spectroscopic techniques, combined with multivariate statistical tools, have been used to detect and characterize microorganisms in meat (Al-Holy et al., 2006; Grau et al., 2011). The HSI technique has been successfully applied for the detection of total viable count (TVC) and psychotropic plate count (PPC) in various kinds of meat. Feng and Sun, (2013) used NIR-HSI (910-1700 nm) for the determination of TVC in chicken breast fillets and reported TVC values ranging from 3.15 to 8.03 log10 CFU/g. The highest correlation coefficient (R^2 0.94) was obtained using the PLS-R model. The authors ultimately used a PLS-R model to construct prediction maps for chicken fillets that allow the visual appearance of the microbial load on the meat surface during spoilage.

Table 1. Application of Chemometrics in the evaluation of various foodstuffs

Sample	Application	Measuring instrument	Chemometric technique	Reference
Apple	Defects	HSI (400–900 nm)	PCA+LDA	[Lu, 2003]
Citrus	Citrus canker	HSI (400–900 nm)	PCA	[Qin, 2008]
Orange	Defects	HSI (400–1,000 nm)	PCA+BR	[Li, 2011]
Beef	Spoilage	FT-IR (4,000–400 cm^{-1})	ANN	[Ammor, 2009]
Beef	Spoilage	FT-IR (4,000–400 cm^{-1})	PLS-R	[Argyri, 2010]
Chicken	TVC	NIR-HSI (4,000–1,700 nm)	PLS-R	[Feng, 2013]
Cucumber	Chilling damage	HSI (447.3–951 nm)	PCA+FLD	[Cheng, 2004]
Mushroom	Freeze damage	HSI (400–1,000 nm)	PCA+LDA	[Gowen, 2009]
Maize	Fumonisins	Raman (4,000–400 cm^{-1})	KNN+LDA MLR+PLSDA	[Lee, 2013]
Rice	Aflatoxin	NIR (950–1,650 nm)	PLS-R	[Sirisomboon, 2013]
Milk	Brucella spp.	Raman (113–3,186 cm^{-1})	LDA+SVM	[Meisel, 2012]

These visualization maps are also an alternative method for testing the model efficacy. In another study, Barbin et al., (2013) used NIR-HSI to assess the TVC and PPC in stored pork meat at two different temperatures (0°C and 4°C) by using a microbiological plating method. Previous experiments had shown that the maximum microbial load in meat was 10^7 CFU/g (Knox et al., 2008). Since meat is rejected for further use when this value is exceeded, the author selected 10^7 CFU/g to classify fresh (up to 10^7 CFU/g) and spoiled meat (over 10^7 CFU/g). The wavelengths that discriminate fresh meat from spoiled meat are 964 nm (O-H stretching), 1,151 nm (C-H stretching), 1,395 nm (protein content), and 1,634 nm (combination of C-H stretching). These wavelengths are influenced by the microbial load in pork meat. High accuracy (94%) for the classification of fresh and spoiled meat was obtained by LDA. In addition, the correlation coefficient (R^2) obtained with the PLS model was 0.93 for both TVC and PPC. The contamination map obtained with the PLS model shows that the contaminated spots on the pork meat were developing in parallel with the days of storage.

E. coli is a major bacterium normally residing in the intestine of humans, and human infection by this pathogen is likely through the consumption of contaminated water or food products (Siripatrawan et al., 2010), especially raw vegetables and undercooked ground beef. *E. coli* O157:H7, which is an enterohemorrhagic serotype species of *E. coli*, is readily found in ground beef and is associated with diarrhea and kidney failure (Boken et al., 2013). Recently, FT-IR spectroscopy in the range of 3,600 to 700 cm^{-1} was applied to detect *E. coli* O157:H7 in ground beef (Davis et al., 2010). In that study, ground beef was inoculated with various quantities of living and heat-treated *E. coli* O157:H7 cells; then, the filtration-FT-IR and immunomagnetic separation (IMS)-FT-IR (4,000-650 cm^{-1}) method was used for the detection of bacteria in the meat. The authors found that the absorbance region between 1,800 and 900 cm^{-1} provided the characteristics of the bacteria. Filtration-FT-IR and IMS-FT-IR showed 100% clear separation between the contaminated and the control ground beef spectra at 1 h and 4 h, respectively, with a detection limit of 10^5CFU/g. In contrast, the conventional plating method needed 48 h of incubation. Therefore, the authors concluded that, when compared to the conventional plating technique, these methods are faster and simpler. Finally, the PLS model predicted the number of *E. coli* O157:H7 cells in ground beef with R^2 of 0.99 (Filtration-FT-IR method) and 0.97 (IMS-FT-IR method).

A different study compared the performance of both FT-IR (4,000 to 650 cm^{-1}) and Raman spectroscopies in evaluating microbial spoilage in minced beef stored under two different packing conditions: aerobic packing and modified atmosphere packing (MAP) (Argyri et al., 2011). Aerobically packed minced beef contained *Pseudomonas* spp., *Brochothrix thermosphacta*, Enterobacteriaceae, lactic acid bacteria (LAB), yeasts, and molds, while MAP packing delayed or suppressed the growth of these pathogens (Ellis, 2001; Ercolini, 2006). The sensory evaluation revealed that the shelf life of meat under aerobic conditions was 60 h, while under MAP storage it was 72 h. The FT-IR and Raman data, combined with SVM and PLS, gave a better prediction of the microbial counts, with the highest predicted R^2 of 0.83 (TVC), 0.81 (*Pseudomonas* spp. bacteria), 0.83 (LAB) for FT-IR data, and 0.72 (TVC), 0.74 (LAB), 0.78 (sensory) for Raman data. Alexandrakis et al., (2012) utilized both NIR (400-2,498 nm) and FT-IR spectroscopies (4,000-800 cm^{-1}) to investigate the spoilage of intact chicken breast muscles stored under aerobic conditions at 4°C for 14 days. The PLS-DA yielded a classification accuracy of 87.5% (storage days: between 0 and 4 day) and 100% (storage days: between 0 and 8 day; 8 and 14 day) for NIR data as well as FT-NIR data.

The HSI technique has also been successfully applied for online detection of fecal contamination in poultry products (Park, 2011; Yoon, 2010). The improper slaughtering and processing of poultry meat can leave residues of feces and ingesta inside the gastrointestinal tract of the bird, resulting in a primary cause of foodborne illness in humans. Park et al., (2011) used line-scan VIS/NIR hyperspectral imaging for the online detection of poultry fecal contamination within the range of 400-1,000 nm. The system processing speed was 140 birds/min, and the technique can detect small amounts (up to10 mg) of feces and ingesta in the duodenum, cecum, and colon. In addition, the Vis/NIR technique (450-1,680 nm) was used for the classification of ingesta and fecal contamination in poultry processing equipment surfaces (Chao et al., 2008). In this study, a classification model was developed for differentiation of fecal and ingesta contaminant spectra, bare rubber surface spectra, and bare stainless steel surface spectra for poultry classification. The visible and NIR region were adequate for detection of 100% of the fecal and ingesta contaminants. The bare stainless steel surfaces were also differentiated from the contamination samples and the classification result of bare rubber belt surfaces was also satisfactory.

Detection of defects in fruits and vegetables

The occurrence of defects or contamination is an important factor impacting the quality and economic value of fruit and vegetables (Lu, 2003; Gamble, 2010). Bruising is a major defect, appearing on the fruit surface, which results from external forces. It also causes physical and chemical changes in the texture, color, and sugar content of fruits (Boydas, 2014). In addition, bruised areas are more prone to bacterial infection. Chilling injury is another most common defect observed on the fruit cell membrane, which arises because of unsuitable storage conditions or harmful environment conditions (Elmasry et al., 2009). Chilling injury leads to symptoms such as a water-soaked appearance, mushy texture, and failure to ripen normally (Cheng et al., 2004).

Spectral techniques are now widely used for the non-destructive assessment of defects and contamination in fruits and vegetables. Previously, the Vis/NIR HSI system was built in the spectral range of 400-1,000 nm for the detection of bruises on Golden delicious apples (Xing et al., 2005). PCA was used to enhance the bruise features and for data dimension reduction. The authors suggested that the 558 nm and 678 nm bands were related to the typical bruise characteristics: browning and chlorophyll loss. The optimum wavelengths selected from the PCA for the detection of bruises were centered at 558, 678, 728, and 892 nm, and good classification accuracy of 93.55% (sound) and 86.5% (bruised) was obtained; the score images generated from the PCA were also capable of determining the apples samples as sound or bruised.

HSI in the range of 400-1,000 nm has been used to investigate chilling injury in Red Delicious apples (Elmasry et al., 2009). The ANN model was developed for wavelength selection, firmness prediction, and classification of the apples. Five optimal wavelengths (717, 751, 875, 960, and 980 nm) were selected by the ANN model for assigning the input nodes. The model predicted the firmness with an R^2 value of 0.92 and the classification accuracy was 100% for normal and 96.9% for injured samples. Citrus canker is the severest disease that affects the peel of the citrus fruit; therefore, several recent studies have been conducted using the HSI technique to detect peel defects in fruits (Balasundaram et al., 2009). Qin et al. (2008) used the HSI technique (400-900 nm) coupled with PCA and the threshold method for detecting canker lesions on Ruby Red grapefruit (citrus variety) surfaces and presented an overall classification accuracy of 92.7% for citrus canker detection. Qin et al. (2009) also used the HSI technique, coupled with the spectral information divergence (SID) algorithm, for the detection of citrus canker on grapefruit, which increased the overall classification accuracy to 96.2%. In addition, external insect infestations in jujube fruit were investigated using the HSI technique in the range of 400-720 nm (Wang et al., 2011). Stepwise discriminant analysis was used to differentiate the insect damaged jujubes from normal ones and an overall classification accuracy of approximately 97.5% was obtained. The HSI technique (400-700 nm) combined with fluorescence and image processing was also used for the investigation of cuticle (crack) defects in cherry tomatoes (Cho et al., 2013). In that study, the authors implemented the analysis of variance (ANOVA) method and obtained the highest F value at the waveband of 670 nm between the sound and defective areas of the cherry tomatoes. Finally, the F value and threshold method differentiated the sound and defective areas. The model yielded almost 99% discriminant accuracy and the image processing task showed excellent separation of the defective areas from the sound areas of the cherry tomato.

Most recently, the HSI technique operated in the transmittance mode has been used for the detection of insect-damaged soybeans within the range of 400-1000 nm (Huang et al., 2013). The support vector data description (SVDD) algorithm was used to classify normal and insect-damaged soybeans. The classification accuracies were 95.6% (normal samples) and 87.5% (insect-damaged) respectively, with an overall classification accuracy of 95.6%. Pickling cucumbers are more prone to internal defects due to transportation and postharvest handling procedures (Miller et al., 1995). The HSI method (400-1000 nm) operated in the transmittance mode has been used to discriminate normal and defected pickling cucumbers (Ariana and Lu, 2010). The overall classification accuracy of the PLS-DA model was 94.7% between normal and defective groups when using four wavebands (745, 805, 965, and 985 nm). Finally, the authors constructed segmented images that provided visual observation of water-soaked lesions in the defected cucumbers, which are visually different from normal cucumbers.

Spinach is the most common green leaf, widely used as vegetable and salads purpose. *E. coli* is the major bacterium commonly found on fresh spinach leaves and is associated with food-borne illness caused by the undercooking of these leaves. The HSI technique has been successfully used in the range of 400-1000 nm for the detection of *E. coli* in freshly packaged spinach (Siripatrawan et al., 2011). PCA was applied for the reduction of the MLP neural network on back propagation and was used to predict the number of *E. coli* cells on the spinach leaves. A good coefficient of determination (R^2 = 0.97) was obtained from the MLP model for the prediction of the number of *E. coli* cells on packaged spinach. The author also generated prediction map from the ANN model that was able to visualize the number of pixels contaminated with *E. coli* and the color of the mapped image corresponds to the number of *E. coli* (expressed as Log (CFU/g)). This generation of a prediction map is an alternative method for interpretation of the HSI data and for testing the model efficiency. In addition, it provides an easy visualization of the microbial contaminated regions on the samples by normal eye.

Detection of contamination in dairy products

Recently, milk products were contaminated with an industrial chemical named "melamine," which is frequently used in industries for the manufacture of plastic, paperboard, flooring, and dishes. The major outbreak of melamine contamination was noticed when several animals (cats and dogs) fell severely ill and died in United States after the intake of melamine adulterated milk and feed materials (Gossner et al., 2009; Andersen et al., 2008; Brown et al., 2007) imported from China. Melamine from contaminated products accumulates in the body and causes kidney stones and renal failure. Traditional methods for melamine detection such as gas chromatography (Miao et al., 2009), mass-spectrometry (Liu et al., 2012), HPLC (Venkatasami and Sowa, 2010), and fluorescence polarization immunoassay (Wang et al., 2011) are time consuming. NIR is an alternative tool for the rapid detection of melamine in dairy and food products. Recently, NIR reflectance spectroscopy in the spectral range of 12,000-3,800 cm^{-1} was used for the detection of melamine contamination in soybean-based meals (genetically and non-genetically modified) containing different amounts of melamine. The authors obtained a distinct melamine peak at 6,800 cm^{-1}. The PLS and PCR analyses showed good coefficient of determination (R^2 = 0.89-0.99), for the prediction of melamine concentration in soybean-based meals. Lu et al., (2009) used NIR spectroscopy for the detection of pure melamine in milk powder. The author analyzed the NIR data with the LS-SVM and PLS methods; LS-SVM displayed a good classification accuracy (100%) for the detection of pure melamine from milk powder, and the detection limit was 1 ppm. In another study, a portable Raman spectrometer (1-1,500 cm^{-1}) was tested to detect melamine in liquid milk (Zhang et al., 2010). This study recorded the peaks of solid melamine at 382, 584, 678, and 983 cm^{-1}, which were related to the triazine ring. An excellent linear relationship (R^2 = 0.99) was obtained between the Raman spectrum and melamine concentration, and the detection limit was 0.5 μg/mL of melamine in liquid milk.

Apart from melamine contamination, pathogenic microorganisms have also been the causative agents of foodborne illnesses; therefore, the detection of pathogens in dairy products is important to address the safety concerns of public health. The microbiological plating method or molecular genetic methods currently being used for pathogen detection in dairy products are time consuming and labor-intensive. However, vibration spectroscopy is a rapid and successful technique for pathogen identification. *Brucella* causes "brucellosis" in humans by contacting with an infected animal or by consumption of unpasteurized milk. Meisel et al. (2012) used micro-Raman spectroscopy (113-3,186 cm^{-1}) for the detection of *Brucella* spp. in contaminated milk. The authors reported overall classification accuracy was greater than 90% for *Brucella* characterization using the SVM and LDA models. In addition, major peaks in the Raman spectra were influenced of course by the presence of the bacteria. In another study, *Pseudomonas* spp. and *E. coli* pathogens in milk were investigated using two different isolation methods: BDC (buoyant density centrifugation) and MC (Milk clearing), and Raman spectroscopy was used later to investigate the compatibility of both these isolation methods for the identification of bacteria in milk (Meisel et al., 2011). The authors found that the BDC method more robustly correlated with the Raman spectra for the classification and identification of the bacteria, with a classification accuracy of 91%, while the MC method showed an accuracy of 78%.

Detection of damage in cereal grains

Spectroscopic techniques are becoming a powerful tool for grain characterization and safety assessment. Recently, various applications of spectroscopy have been reported for grain quality analysis, which includes fungal detection, damage detection, and variety classification (Tallada et al., 2011, Shahin et al., 2011). Aflatoxin is a mycotoxin produced by the secondary metabolites of the fungus *Aspergillus flavus*, which severely affects agricultural commodities (Tripathi and Mishra, 2009; Wu et al., 2012) particularly corn, soybeans, wheat, rice, and nuts (Fuller et al., 1977 ; Gloria et al., 2006; Shortwell and Hesseltine, 1974; Steiner et al., 1992). Toxins produced in the grains decrease their nutrient content, which is directly related to economic loss and impaired health in humans and animals that consume them.

Recently, Lee et al., (2014) investigated aflatoxin in ground maize samples using Raman spectroscopy within the range of 200-3,500 cm^{-1}. Samples with five different aflatoxin concentrations were used for Raman and HPLC measurements. Spectral differences were observed in contaminated samples around 400-620 cm^{-1}, 750-1,200 cm^{-1}, and 1,400-1,800 cm^{-1} owing to the presence of aflatoxin. The LDA model showed almost 100% classification accuracy between normal and contaminated groups, while the PLSR model predicted good R^2 (0.94-0.95) for aflatoxin concentration. Tripathi and Mishra (2009) demonstrated the potential of the FT-NIR spectroscopy technique (12,000-4000 cm^{-1}) for the estimation of aflatoxin B1 (AFB_1) in red chili powder. In this study, HPLC and thin layer chromatography (TLC) were performed to compare the FT-NIR performance. The PLS analysis yielded a high R^2 (0.96) for the prediction of aflatoxin concentration in chili powder. In addition, the furocoumarin ring structure (corresponding to the C-H stretching, 6923.22 cm^{-1}) correlates with the phenolic content of the sample and aromatic ring structure (corresponding to the C-H symmetrical stretching, 4262.37 cm^{-1}) correlates with the alkaloidal content of the sample.

Fusarium disease is also a serious problem for wheat, barley, and oat seeds (Bauriegel et al., 2011; Bauriegel and Herppich, 2014; Draganova et al., 2010). A recent study by Shahin and Symons (2011) reported the detection of Fusarium-damaged kernels (FDK) in Canada western red spring wheat using the Vis/NIR HIS technique in the range of 400-1,000 nm. Optimal wavebands were selected by PCA, which were used in the LDA; sound and contaminated samples were classified with an overall accuracy of 92%. Mildew is another fungal contamination found in wheat crops and is caused by the growth of *Cladosporium* spp. and *Alternaria alternata* under wet or humid conditions. Shahin et al. (2014) reported on the application of Vis/NIR HSI (400-1,000 nm) and FT-NIR (1,000-2,500 nm) spectroscopies for the detection of mildew damage in red winter wheat. The PLS model provided the R^2 value of 0.95 in the range of 450-950 nm, and the R^2 value of 0.87 in the range of 1,000-2,500 nm. In addition, the highest mildew level classification accuracy was 96%. On the other hand, use of the HSI technique (1,000-1,600 nm) and linear and quadratic discriminant analysis (Singh et al., 2009) allowed the correct classification of 85-100% of healthy and insect-damaged wheat kernels (damaged by *Sarocladium oryzae*, *Rhyzopertha dominica*, *Cryptolestes ferrugineus*, and *Tribolium castaneum*) .

Conclusions

This review describes the various applications of spectral modalities, specifically hyperspectroscopy and vibrational spectroscopies (FT-IR and Raman spectroscopy), for the detection of contaminations and defects in agro foods. In contrast to the conventional methods, which are time-consuming, labor intensive, expensive, and require destruction of the sample, these spectral modalities coupled with chemometric analysis are non-destructive, accurate, and convenient for quantitative and qualitative analysis of food and agricultural products. The three-dimensional feature of hyperspectral imaging provides more accurate information of the sample, and vibrational spectroscopies reveal the vibrational behavior of the molecular bonds present in the samples. However, proper calibration of the instruments is challenging during measurement; therefore, various pre-preprocessing techniques and chemometric analyses are used to handle the spectra for robust models. Although these spectral techniques provide useful information regarding the samples, they are quite expensive. Therefore, the development of low-cost and simple instruments is required to meet industrial needs.

Conflict of Interest

The authors have no conflicting financial or other interests.

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