The Canadian Society for Bioengineering
The Canadian society for engineering in agricultural, food, environmental, and biological systems.

La Société Canadienne de Génie Agroalimentaire et de Bioingénierie
La société canadienne de génie agroalimentaire, de la bioingénierie et de l'environnement

CSBE | SCGAB

Paper No. 06-189

Near-infrared spectroscopy: Applications in the grain industry

C.B. Singh

Graduate Student, Department of Biosystems Engineering, University of Manitoba, Winnipeg, MB, Canada R3T 5V6

J. Paliwal

Assistant Professor, Department of Biosystems Engineering, University of Manitoba, Winnipeg, MB, Canada R3T 5V6

D.S. Jayas*

Associate Vice-President (Research), Distinguished Professor, and Canada Research Chair in Stored-Grain Ecosystems, Department of Biosystems Engineering, University of Manitoba, Winnipeg, MB, Canada R3T 5V6

N.D.G. White

Senior Research Scientist, Agriculture and Agri-Food Canada, Cereal Research Centre, Winnipeg, MB, Canada R3T 2M9

*Corresponding author: Digvir_Jayas@Umanitoba.ca

Written for presentation at the
CSBE/SCGAB 2006 Annual Conference
Edmonton Alberta
July 16 - 19, 2006

Abstract. *Grains are among the most important staple foods for the world's population. There is an increasing demand from consumers for the highest quality of food products and zero-tolerance for grain contamination. Grain quality is affected mainly by moisture content; soundness and vitreousness of the kernels; amount of foreign material; and presence of fungi, insects, and mites. The current visual methods for grain quality estimation are subjective and time consuming. The grain industry is in need of an automated, economical, and rapid means of grain quality estimation. The technique of near-infrared spectroscopy (NIRS) has demonstrated the potential to measure most of the grain quality attributes in real- time and it has been proven to be a fast, reliable, accurate, and economical analytical technique. Though the NIRS technology has been applied for quality analysis of food and bio-material, its real-time applications have been restricted due to complex spectra; highly overlapping, broad, low absorption band and there is a need for detailed calibration. Precise and robust NIRS calibration models can be developed using wavelet transform and artificial neural network (ANN). This paper reviews the applications of NIRS for grain quality evaluation.*

Keywords: *Near-infrared spectroscopy, grain quality, reflectance and transmittance characteristics, multivariate analysis.*

Introduction

There is an increasing demand from grain buyers for the highest quality of grain, as a result of tremendous pressure from food manufacturers, their own competitors in the grain market, and globalization of the grain industry. Grain quality has been defined by several factors such as moisture content, bulk density, kernel size, kernel hardness, vitreousness, kernel density, total damaged kernels, fungal infection, mycotoxins, insects, mites, and foreign material. Stored grain can have losses in both quantity and quality during storage as a result of development of insect and mite infestations and mould infection. Deterioration and contamination results in downgrading grain and lower market value due to insect parts, odors, molds, increase in free fatty acid, heat damage, toxicity, poor milling and baking quality. The insects cause losses by destroying large quantities of cereals (rice, wheat, and corn), legumes (beans, lentils, and peas), milled cereal products (flour, bran, and macaroni), pet foods, dried fruits, dried vegetables, cheese, nuts, candy, and other food materials. Feeding of whole grains by the insects causes weight loss, fungal growth, and quality loss which results in increased free fatty acid levels (Sinha and Watters 1985). There is an increasing trend in the processed food industry to increase the nutritional value of processed food. Therefore, cereals are analyzed for composition of starch, protein, moisture and a small portion of lipids and fiber which affect the quality of end use products. At present, manual inspection or chemical analytical methods are widely used for grain quality estimation at grain handling facilities, which are not efficient and time consuming. Therefore, a fast and reliable method is needed for grain quality estimation in real time. The near-infrared spectroscopy (NIRS) has evolved as a fast, reliable, accurate and economical technique available for grain quality analysis (Kim et al. 2003). This multi-analytical technique is rapid, requires very little or no sample preparation and several parameters can be estimated simultaneously. The objective of this article is to review the applications of NIRS technique in grain quality analysis.

Principle of spectroscopy

Spectroscopy is the study of physical characteristics of atoms or molecules by using electromagnetic radiation in the form of absorption, emission, or scattering by molecules.

Electromagnetic radiation is an energy wave composed of both electric and magnetic field properties. These properties interact with matter to form a spectrum. Electromagnetic radiation also has both wave and particle characteristics. When light passes through matter it may be absorbed by atoms or molecules and then molecules are excited to higher energy levels depending on the wavelength and intensity of the light source. This process is called absorption. A part of electromagnetic radiation passing through a material may scatter in other directions. These atoms or molecules which are excited to higher energy levels can return to lower energy levels by radiating energy (emission). These energy levels can be distinguished by integers called quantum numbers. A transition in the energy levels can occur if the appropriate amount of energy is either absorbed or emitted by the atoms or molecules. According to Planck's theory this transition energy change can take the form of electromagnetic radiation and the frequency of radiation is related to energy change ($\Delta E = hv$, where ΔE is energy change, *h* is Planck's constant and *v* is radiation frequency). An absorption spectrum can be produced by collecting the radiation after its interaction with the material. The frequency and wavelength of light source are interrelated ($v = c/\lambda$, where c is speed of light in vacuum, 3×10^8 m/s and λ wavelength of light source). A molecule in space can have several forms of energy such as vibrational, rotational, electronic and translational energy. Vibrational energy is the result of periodic displacement of atoms from their equilibrium position and rotational energy is the result of rotation about a center of gravity. In NIRS vibrational energy is mainly considered.

Near-infrared spectroscopy measures the wavelength and absorption of near-infrared (NIR) light by a material. Near-infrared region is defined as the wavelength region from 700 to 2500 nm (Wavenumber 14300 to 4000 cm^{-1}), between the visible light and the infrared light region (Osborne et al. 1993). In NIR instruments, signal to noise ratio is very high (10000:1) (Hans 2003). The NIR spectrum shape is characterized by overtone and combination bands of fundamental vibrations occurring in the mid and far infrared region. Due to complex molecular structures of most organic compounds, the resulting spectra are the result of many overlapping peaks and valleys. The NIR spectroscopic technique works on the principle that unique chemical composition causes molecules to absorb light in the NIR region and vibrate at unique frequencies (Murray and Williams 1990). Reflected or transmitted light is collected by a spectrometer that measures energy absorbed by the sample. Near-infrared spectra obtained from the absorption at multiple wavelengths can be related to the concentration of a particular constituent of the sample.

Calibration and data analysis

The NIR instrument must be calibrated prior to its use for quantitative measurement. Calibration experiment involves collecting a set of reference data by some other method (e.g. chemical analysis), which should contain all chemical and physical variations to be expected in the samples from an unknown population. The NIR instrument determines chemical and physical composition of the food material by measuring log (1/R) values, where R is reflectance. Then a relationship between reference data and log (1/R) values of a set of samples of known composition is established by regressing reference data to the spectral data (log 1/R). The essential information from spectra is extracted by using chemometric techniques such as multi-variate analysis. Multi-variate analysis relates spectral parameters to reference data which is capable of predicting the characteristics and properties of unknown samples (Blanco and Villarroya 2002). Before spectral analysis, the spectral data are pretreated by using normalization, derivatives (usually first or second), multiplicative scatter correction (MSC), standard normal variate (SNV), de-trending (DT) or a combination of these (Wang et al. 1999b; Blanco and Villarroya 2002; Blanco et al. 2005). The data pretreatment reduces baseline effect, nonlinearity and particle size effect on the spectra. A number of multi-variate calibration methods such as principal component analysis (PCA), partial least squares (PLS), and artificial neural network (ANN) are used for calibration of NIR instruments (Roggo et al. 2003; Blanco et al. 2005). Spectral data are used in PCA analysis and then calibrated data are related to principal components using multiple liner regression (MLR). In the PLS technique linear combinations of the original spectral data are used to construct a small number of factors and then these factors are used to derive a prediction equation using regression. Artificial neural networks have been used extensively in NIR spectroscopy as an alternative to partial least squares (PLS) and multiple linear regression (MLR) (Gordon et al. 1998). In ANN, each neuron (unit) acts as a simple processing unit that transforms input signal in a non-linear way. They are connected to a bunch of other neurons through which electrical signals can cross from one neuron to another. This structure is called a neural network. Computations are based more on discriminant-based functions looking more for spectral similarity to those in the database. Artificial neural network techniques have the advantage that they can handle non-linearity between the spectral data and the constituents and offer multiple opportunities for optimization whereas a PLS or MLR calibration offer only one option. Researchers have proposed methods to improve generalization of ANNs when dealing with spectral data (Wang and Paliwal 2006).

In recent years, the advent of wavelets has provided an option to the traditional signal compression and analysis problems using Fourier transform (FT). The wavelet transform compresses the spectral data, separates the overlaping bands, and eliminates the signal/image noise without any considerable loss of infromation. A wavelet is defined as a family of functions derived from a basic function, called the wavelet basis function, by dilation and translation. Wavelet transform (WT) is a projection operation of a signal onto the wavelet. Although analogous to FT, WT uses one of the several available wavelets as the basis function. Therefore, a large number of basis functions are available in WT as opposed to only two (i.e. sine and cosine) for FT. The most outstanding characteristic of the WT is the localization property in both time and frequency domains, while FT is localized only in the frequency domain. With proper identification, WT may be used to zoom in and out at any part of the signal at any frequency and a complex signal can be decomposed into its different frequency components (Prasad and Iyengar 1997). Since a spectral signal is generally composed of a baseline, noise, and the chemical signal; it is not difficult to use WT by removing the high-frequency part from the signal for denoising and smoothing and by removing the low-frequency part for baseline correction. Although in biological engineering WT has been successfully used in the areas of remote sensing and soil and water conservation, its potential has not been fully explored and utilized in predicting the functional constituents of grain. Chen et al. (2002) used WT to predict oil content in instant noodles and found the technique performed better than first and second derivatives of the spectra. The performance of the developed NIRS calibration models is evaluated by standard error of calibration (SEC); standard error of cross validation (SECV); standard error of performance (SEP); coefficient of determination (R^2); linear correlation coefficient (r) between reference values and values estimated by prediction models; and discrimination index (Miralbes 2004).

Applications

The NIR spectroscopy is widely used in the grain industry for determining grain quality. The scope of NIR application in food and grain quality analysis is very high. In the following sections the main applications of NIRS in the grain industry are described.

Hardness measurement

Wheat grain hardness is a quality characteristic that defines or determines milling characteristics and its end use (Slaughter et al. 1992). Delwiche and Norris (1993) classified hard red wheat classes by analyzing NIR diffuse reflectance spectra from ground wheat samples. A linear discriminate function based on protein content, NIR-hardness, and protein and hardness classified the wheat samples into hard red winter (HRW) and hard red spring (HRS) wheats. Year-to-year compositional changes in these constituents resulted in lower classification accuracy. Delwiche et al. (1995) applied full NIR reflectance spectra to the bulk wheat samples to overcome the yearly effect and examined four types of classification algorithms: multiple linear regression (MLR), PCA with Mahalanobis distance, PLS analysis, and ANN model. The ANN model gave the highest classification accuracy (95-98%) among the four models investigated. These models were not able to distinguish the mixtures of various classes and were limited to classify wheat only into HRW and HRS classes. Maghirang and Dowell (2003) measured hardness of bulk wheat by using single-kernel visible and near infrared reflectance spectroscopy. The reflectance spectra were related to protein, starch, and color differences. Use of both visible and NIR reflectance spectra, and mass averaging of spectra in the PLS analysis improved hardness classification. The prediction model correctly classified samples with 72-100% accuracy and mixtures containing high hardness hard wheat gave relatively better classification (95% to 100%). Guillemero et al. (1996) measured the hardness of maize by using NIR transmittance spectroscopy. Their study indicated the feasibility of analyzing endosperm hardness by determining whole kernel absorbance at 860 nm.

Vitreousness determination

Vitreousness of hard wheat is the glossy or shiny appearance. Vitreousness affects the milling performance (Semolina yield) and quality of some products from semolina (e.g. pasta). It is an indicator of hardness and high protein content and considered by the wheat industry as milling and cooking quality parameters. Dowell (2000) used NIR spectroscopy to classify single wheat kernels into vitreous and non-vitreous classes. Classifications of obviously vitreous and non-vitreous kernels were in good agreement with those of inspectors. However, classification accuracy reduced up to 75% when difficult to classify vitreous and non-vitreous kernels were included in the analysis. In this study the effect of wheat crop year on model performance was not investigated as only samples from one crop year samples were used. Wang et al. (2002) sub-classified HRS wheat in dark hard vitreous (DHV) and non-dark hard vitreous (NDHV) kernels using visible/near-infrared spectroscopy by collecting spectra from single DHV and NDHV kernels using a diode-array spectrometer and transforming the reflectance spectra in to color space. The HRS wheat samples included checked, cracked, sprouted, and bleached kernels. Their PLS model gave good prediction results (97.1-100%) but failed to classify bleached kernels. Light scattering, protein content, kernel hardness, starch content, and kernel color contributed to the classification of DHV and NDHV kernels. The classification accuracy may be affected by the subjectivity involved in the reference determination of vitreousness by a panel.

Grain color classification

Grain color and appearance affects the market value of the grain and misclassification of color classes results in lower grain quality and a loss of monetary value. Wheat kernel color varies from light yellow to red brown and is affected by red pigment in the seed coat and growing condition. Red wheat and white wheat have different milling, baking, taste properties, and different visual characteristics (Dowell 1997). Wang et al. (1999a) classified 6 classes of wheat samples in to red and white wheat using NIR reflectance spectra in of 500-1700 nm. Both PLS and MLR based calibration models classified wheat kernels with highest accuracy of 98.5 and 98.1%, respectively. The wheat kernel size affected the visible and NIR reflectance spectra, thus color classifications and this affect was reduced by first and second derivative pre-treatments.

This size affect can also be eliminated/reduced using pre-treatment methods such as MSC and first or second derivative with MSC (Wang et al. 1999b).

Classification of bulk cereals

Due to variations in climatic, harvest, and growing conditions grains from different growing regions may have diversity in moisture, foreign material, color, morphology, and chemical characteristics. These factors affect the quality of the grain and crop value. Mohan et al. (2005) used visible and near-infrared reflectance characteristics for classification of bulk grain samples of seven cereals namely, Canada Western Red Spring (CWRS) wheat, Canada Western Amber Durum (CWAD) wheat, Canada Western Soft White Spring (CWSWS) wheat, 2–row barley, 6–row barley, oats, and rye. Using five features, the linear parametric and back propagation neural network (BPNN) based calibration models correctly classified 99.5% of the bulk grain samples. Moisture, foreign material and growing locations affected the reflectance characteristics of CWRS wheat when treated as a single entity; but when the variables were segregated as individual classes, cereals were correctly classified. Delwiche and Masie (1996) classified kernels of different cultivars using visible and NIR reflectance characteristic from single kernels. They used PLS and MLR techniques to develop binary calibration model for various combinations of two wheat classes selected from five wheat classes (hard white, HRS, HRW, soft red winter (SRW), and soft white). They developed a two class model and also a five-class model using a cascade of binary comparisons similar to the two class model. Two-class model achieved accuracy of 99% when red and white wheat classes (contrast in color) were classified. But this model could not correctly classify wheat classes of similar colors (e.g. HRW vs. SRW) and model accuracies declined to 78-91%. Accuracy of a five-class model ranged from 65% for SRW wheat to 92% for soft white wheat. Mohan et al. (2004) studied diffuse reflectance characteristics of bulk oilseeds, specialty seeds and pulses by analyzing their reflectance characteristics in ultra-violet, visible and NIR region, and extracted 156 ratio, 155 slope and 154 slope-ratio features from reflectance spectra. They used BPNN to determine weights of individual features and selected the top 20 features for classification accuracy. Ratio features and the slope-ratio features gave better classification results than the slope features. The majority of features were from the visible and NIR region. They achieved 100% classification accuracy using both non-parametric classifier and BPNN.

Identification of damaged grain

Heat, insect, and fungal damaged grain affect the quality of whole grain and lower the market value. Heat damage results in protein denaturation, germination loss, and reduces processing quality. Wang et al. (2004a) classified healthy and fungal-damaged soybean seeds and differentiated among various types of fungal damage using NIR spectroscopy in the wavelength region of 400 to 1700 nm. The two-class PLS model achieved classification accuracy of more than 99%. The ANN model yielded higher classification results than the PLS model and correctly classified healthy seeds, *Phomopsis, Cercospora kikuchii*, soybean mosaic virus (SMV), and downy mildew damaged seeds with 100, 99, 84, 94, and 96% accuracy, respectively. Wang et al. (2001) evaluated the use of NIR reflectance spectroscopy to identify heat damaged wheat kernels. They found that light scattering and color were the major contributor to the spectral characteristics of heat-damaged kernels. The PLS based calibration model using 750 to 1700 nm wavelength region identified all damaged and umdamaged kernels in both cross-validation and prediction sample sets. A two-wavelength model based on color differences in the damaged and undamaged kernels classified more than 96% wheat kernels accurately. In this study only two wheat classes HRS and HWW were used for analysis; more classes with larger sample size should be included in model development for industrial application. Delwiche and Hareland

(2004) developed a semi-automated system to identify scab-damaged wheat kernels based on NIR reflectance (1,000-1,700 nm) of single kernels. Scab infection results in lower crop yield, poor flour quality, and development of a mycotoxin called deoxynivalenol (DON). Using linear discriminant and nonparametric (*k*-nearest-neighbor) analysis, they achieved highest classification accuracy of approximately 88% in cross-validation) and 97% in the test set. Though this classification accuracy is low this technique has potential for commercial inspection of fungal damaged grain and needs further investigation.

Moisture content determination

Moisture content is considered the most important physical characteristic of grain in the grain grading system. It affects moisture migration, mould growth, and insect and mite infestation and the monetary value of grain. Wang et al. (2004b) studied feasibility of applying NIR spectroscopy to determine moisture content of ground wheat. The NIR spectra of ground wheat samples were affected by instrumental stability, sample homogeneity and compactness, moisture content, and particle size. Instrumental noise was eliminated by averaging of spectral data. The PLS model calibrated on the first derivative of averaged spectra provided the best results. Spectral data pre-treatment techniques MSC, SNV, and DT failed due to small sample size. Cogdill et al. (2004) studied the feasibility of an NIR hyperspectral imaging spectrometer for moisture and oil content analysis of single maize kernels. Maize oil content and moisture content were determined by supercritical fluid extraction and oven method, respectively, for reference data. Calibration algorithms were developed using PLS and PCA techniques to predict moisture and oil content. Preprocessing treatments such as standard normal variate, detrending, multiplicative scatter correction, wavelength selection by genetic algorithm, and no processing were compared for their effect on model performance. The PLS based calibration model predicted moisture with a best SECV of 1.20% and relative performance index (RPD) of 2.74. The calibration model predicted oil content with a SECV of 1.38% an RPD of 1.45. They observed that performance and subsequent analysis of the oil calibration need improved methods of single-seed reference analysis. Gribtus and Burns (2006) developed NIR calibration model for moisture content estimation of wheat using wavelet transform. Their calibration model gave high prediction accuracy with SECV of 0.096%, SEP of 0.27, and r^2 of 0.96.

Chemical composition analysis

Chemical compositional analysis of cereal grain and grain products is important for their quality evaluation. Improvement in nutritional composition of the grain enhances the crop value. Berardo et al. (2004) evaluated the carotenoid concentrations in maize by applying NIR spectroscopy and developing calibration model using high performance liquid chromatography (HPLC) data set. Carotenoid concentrations determined by NIR model were in good agreement with those of HPLC method (r^2 value ranged from 0.82 for lutein to 0.94 for zeaxanthin). With precise reference data, an NIR model can determine carotenoids content in maize more accurately compared to that of the conventional chromatographic methods. Wesley et al. (2001) measured protein content (gliadin and glutenin) of wheat flour by NIR spectroscopy and compared the results with a traditional curve fitting method (chromatography). They collected the reference data by determining the gliadin and glutenin contents by size exclusive-high performance liquid chromatography (SE-HPLC) technique and developed a PLS calibration model and compared the results with curve fitting methodology. Pasikatan and Dowell (2004) used NIR spectroscopy to segregate low and high protein wheat seeds. Mbuvi et al. (2001) predicted amylose content in corn of whole and ground corn kernels by applying NIR spectroscopy. The NIR instruments with extended spectral range to the visible region allowed the measurement of pigments such as chlorophyll in immature canola seed (Williams and

Sobering 1993) and carotenoids in wheat (McCaig et al. 1992) by measuring absorbance (reflectance) at specific wavelengths associated with the pigments.

Detection of insects and mites infestation

Detection of internal infestation by insects such as weevils and borers in whole grain is complicated by the presence of hidden immature stages (eggs, larvae, and pupae) inside grain kernels. Samples of grain may appear to be insect-free if no adults are present, when in fact they might be infested by immature stages. Insect species have different chemical composition than those from grain which affects the NIR spectra and internal insect can be detected by NIR analysis. Maghirang et al. (2003) used an automated NIR reflectance system to detect internal infestation in single wheat kernels by live or dead rice weevils at various growth stages. They achieved average classification accuracies of 94%, 93%, 84%, and 63% for sound kernels plus kernels containing live pupae, large larvae, medium-sized larvae, and small larvae, respectively. Dowell et al. (1999) examined the possibility of application of NIR spectroscopy for taxonomic purposes and developed calibration model by PLS and ANN analysis. ANN model correctly identified 99% of test insects as primary or secondary pests and 95% of test insects to genus. They observed that absorption characteristics of cuticular lipids might contribute to the classification accuracy. Karunakaran et al. (2005) used both the soft X-ray and NIR spectroscopy methods to detect insect infestations to evaluate their potential for real-time application by artificially infesting CWRS wheat by rice weevil (*Sitophilus oryzae*) adults. They observed that identification of infestations by both methods increased with the increase in the developmental stage of the insect from larvae to adult stage. X-ray method has the advantage over NIR spectroscopy in small samples where the number of infested or insect-damaged kernels can be counted. The NIR spectroscopy analyzing bulk samples can be applied where the identification of insect species is critical and precise quantification of infestations is not necessary such as for fumigation. Perez-Mendoza et al. (2003) examined the possibility of using NIR spectroscopy for detecting insect fragments in wheat flour and compared the sensitivity and accuracy of the NIR method with that of the current standard flotation method. In wheat flour, defect action level is 75 or more insect fragments per 50 g of flour (FDA, 1988). Near-infrared spectroscopy model was unable to predict insect infestation at this defect action level but identified correctly whether flour samples contained less than or more than 130 insect fragments per 50 g of flour. Paliwal et al. (2004) examined application of NIR spectroscopy for inspection of four different life stages (i.e., eggs, larvae, pupae, and adults) of *Sitophilus oryzae* in artificially infested bulk samples of CWRS wheat. Sound wheat kernels were infested manually with *Rhyzopertha dominica* (Lesser grain borer) to various infestation level (0, 5, 10, 20, 25, 50, 75, and 100% infestation). The PCA and PLS based calibration models differentiated wheat kernels infested with pupae of lesser grain borer from those infested with rice weevil. Their prediction model showed best results for high infestation levels but did not perform well at low infestation levels.

Detection of mycotoxins

When fungi grow on grain, they often produce toxins called *mycotoxins* and contaminate grain. The fungus *Aspergillus flavus* produces very lethal mycotoxins called *aflatoxins*. Aflatoxins can cause diseases such as acute or chronic liver disease and liver cancer. Pearson et al. (2001) studied the possibility of application of transmittance spectra and reflectance spectra for detection of aflatoxin contamination in single whole corn kernels. They obtained reference data by analyzing each kernel for aflatoxin using standard aflatest affinity chromatography procedure and developed calibration models using discriminate analysis and PLS regression. Their classification model correctly classified 95% of kernels as containing either high (>100 ppb) or low (<10 ppb) levels of aflatoxin. However their model was not able to predict the concentration in between 10 to 100 ppb accurately. Dowell et al. (2002) applied reflectance and transmittance spectroscopy to detect fusmonisin in single corn kernels infected with *Fusarium vericillioides*. Fumonisins are mycotoxins produced by the fungi *F. moniliforme, F. proliferatuum* and other fusaria. Kernels with contaminat level greater than 100 ppm were classed as fumonisins positive; where as kernel with level less than 10 ppm were claased as fumonisins negative. Classification accuracy improved by including visible and NIR wavelengths in calibration. Color, chemical composition, and kernel orientation of the infected kernels affected the spectral analysis and contributed to accuracy of classification models.

Direction for further research

The NIRS is a correlative technique in which reference data are regressed against spectral data for future prediction of analytes. NIR model accuracy is heavily dependent on quality of reference data used in the calibration. In certain cases, non-linearity arises between spectral and reference data due to instrumental and physicochemical factors. The complex nature of NIR spectra, noise, and highly overlapping and low absorption band make it diificult to extract relevant information from spectral data. The alternative techniques such as wavelet transform (WT) and ANN offer the possibily of developing more robust NIRS calibration models. A variety of mathematical treatments based on WT, such as wavelet packet transform (WPT), are now available to denoise, smoothen, and improve the signal-to-noise ratio (SNR) of spectral data. WPT is an advancement of WT where decomposition is applied to both the approximation and the detail coefficients. Because of more decomposed components with different frequencies, it is hypothesized that WPT is stronger than WT in segregating noise and resolving overlapping peaks. These treatments need to be tested and evaluated for their ability to determine the functionality of grain. For analysis of spectral data and calibration development the potential of ANNs has not been fully investigated. That is because despite their strengths, ANNs suffer from difficulties in training models with a large number of inputs. This becomes all the more important in hyperspectral analyses because of the shear amount of data. Using different techniques such as a non-random initial connection weight algorithm or local minima avoidance and escape technique these difficulties can be overcome. Improving the generalization capabilities of ANNs is another challenge in this field.

Conclusion

The near-infrared (NIR) spectroscopy technique provides a fast, reliable, nondestructive and accurate assessment of various grain quality attributes and the chemical composition of grain. The application of NIR in grain quality assessment includes grain hardness measurement, color classification, bulk cereal classification, damaged grain identification, moisture content determination, protein content measurement, detection of insect and mites, and fungal infestation. Near-infrared spectroscopy offers the possibility of measuring both physical and chemical properties of the grain in real-time and it has potential for commercial applications in the grain industry. Development of an accurate and robust NIR model requires calibrations which encompass all the variations expected in the physical and chemical parameters and selection of a multivariate technique based on purpose of analysis, characteristics of analytes, and complexity of the NIR instruments. The spectral range, pretreatments, and regression method have to be carefully chosen. The limitations on the NIR applications are due to weak sensitivity of NIR spectra to minor constituents, lengthy calibration procedures, and the problem of calibration transfer between different instruments. Alternative analytical techniques such as wavelet transform and ANN have potential to develop more accurate calibration models with high speed for on-line grain quality analysis.

Acknowledgements

We thank the Natural Sciences and Engineering Research Council of Canada for funding this study.

References

Berardo, N., O.V. Brenna, A. Amatoa, P. Valotia, V. Pisacanea and M. Motto. 2004. Carotenoids concentration among maize genotypes measured by near infrared reflectance spectroscopy (NIRS). *Innovative Food Science and Emerging Technologies* 5: 393-398.

Blanco, M. and I. Villarroya. 2002. NIR spectroscopy: a rapid-response analytical tool. *Trends in Analytical Chemistry* 21(4): 240-250.

Blanco, M., J. Coello, H. Iturriaga, S. Maspoch and J. Pages. 2005. NIR calibration in non-linear systems: different PLS approaches and artificial neural networks. *Chemometrics and Intelligent Laboratory Systems* 50: 75-82.

Chen, B., X. Fu, and D. Lu. 2002. Improvement of predicting precision of oil content in instant noodles by using wavelet transforms to treat NIR spectra. *Journal of Food Engineering* 53:373-376.

Cogdill, R.P., C.R. Hurburgh, G.R. Rippke, S.J. Bajic, R.W. Jones, J.F. McClelland, T.C. Jensen and J. Liu. 2004. Single kernel maize analysis by near-infrared hyperspectral imaging. *Transactions of the ASAE* 47(1): 311-320.

Delwiche, S.R. and D.R. Massie. 1996. Classification of wheat by visible and near-infrared reflectance from single kernels. *Cereal Chemistry* 73(3): 399-405.

Delwiche, S.R. and G.A. Hareland. 2004. Detection of scab-damaged hard red spring wheat kernels by near-infrared reflectance. *Cereal Chemistry* 81(5): 643-649.

Delwiche, S.R. and K.H. Norris. 1993. Classification of hard red wheat by near-infrared diffuse reflectance spectroscopy. *Cereal Chemistry* 70: 29-35.

Delwiche, S.R., Y.R. Chen and W.R. Hruschkha. 1995. Differentiation of hard red spring wheat by near-infrared analysis of bulk samples. *Cereal Chemistry* 72(3): 243-247.

Dowell, F.E. 1997. Effect of NaOH on visible wavelength spectra of single wheat kernels and color classification efficiency. *Cereal Chemistry* 74: 617-620.

Dowell, F.E. 2000. Differentiating vitreous and nonvitreous of durum wheat kernels by using near-infrared spectroscopy. *Cereal Chemistry* 77(2): 155-158.

Dowell, F.E., J.E. Throne, D. Wang and J.E. Baker. 1999. Identifying stored-grain insects using near-infrared spectroscopy. *Journal of Economic Entomology* 92(1): 165-169.

Dowell, F.E., T.C. Pearson, E.B. Maghirang, F. Xie and D.T. Wicklow. 2002. Reflectance and transmittance spectroscopy applied to detecting fumonisin in single corn kernels infected with *fusarium verticillioides.* *Cereal Chemistry* 79(2): 222-226.

FDA (Food and Drug Administration). 1988. Wheat flour adulterated with insect fragments and rodent hairs. Compliance Policy Guides. Processed Grain Guide 7104.511 (Chapter 4).

Gordon, S.H., B.C. Wheeler, R.B. Schudy, D.T. Wicklow and R.V. Greene. 1998. Neural network pattern recognition of photoacoustic FTIR spectra and knowledge-based techniques for detection of mycotoxigenic fungi in food grains. *Journal of Food Protection* 61(2):221-230.

Gributs, C.E.W. and D.H. Burns. 2006. Parsimonious calibration models for near-infrared spectroscopy using wavelets and scaling functions. *Chemometrics and Intelligent Laboratory Systems.* Article in Press.

Guillermo, H.E., J.L. Robutti and F.S. Borras. 1996. Effect of near-infrared transmission-based selection on maize hardness and the composition of zeins. *Cereal Chemistry* 73(6): 775-778.

Hans, B.P. 2003. Analysis of water in food by near infrared spectroscopy. *Food Chemistry* 82: 107-115.

Karunakaran, C., J. Paliwal, D.S. Jayas and N.D.G. White. 2005. Evaluation of soft X - rays and NIR spectroscopy to detect insect infestations in grain. ASAE Paper No. 053139. St. Joseph, MI: ASAE.

Kim, S.S., M.R. Phyu, J.M. Kim and S.H. Lee. 2003. Authentication of rice using near infrared refelectance spectroscopy. *Cereal Chemistry* 80(3): 739-745.

Maghirang, E.B. and F.E. Dowell. 2003. Hardness measurement of bulk wheat by single kernel visible and near-infrared reflectance spectroscopy. *Cereal Chemistry* 80(3): 316-322.

Maghirang, E.B., F.E. Dowell, J.E. Baker and J.E. Throne. 2003. Automated detection of single wheat kernels containing live or dead insects using near-infrared spectroscopy. *Transactions of the ASAE* 46(4): 1277-1282.

Mbuvi, S. W., M.R. Paulsen, M. Bajaj and S.K. Harrison. 2001. Application of near-infrared spectroscopy to predict amylase content in corn. ASAE Paper No. 01-6007. St. Joseph, MI: ASAE.

McCaig, T.N., J.G. McLeod, J.M. Clarke and R.M. Depauw. 1992. Measurement of durum pigment with a near-infrared instrument operating in the visible range. *Cereal Chemistry* 9: 671-672.

Miralbes, C. 2004. Quality control in the milling industry using near-infrared transmittance spectroscopy. *Food Chemistry* 88: 621-628.

Mohan, L.A., C. Karunakaran, D.S. Jayas and N.D.G. White. 2005. Classification of bulk cereals using visible and NIR reflectance characteristics. *Canadian Biosystems Engineering* 47: 7.7-7.14.

Mohan, L.A., D.S. Jayas, N.D.G. White and C. Karunakaran. 2004. Classification of bulk oilseeds, specialty seeds and pulses using their reflectance characteristics. In: *Proceedings of the International Quality Grain Conference, Indiana, USA*. July 19-22. Indianapolis.

Murray, I. and P.C. Williams. 1990. Chemical principles of near-infrared technology. In: *Near-infrared Technology in the Agricultural and Food Industries*, ed. P.C. Williams and K.H. Norris, 17-34. St. Paul, MN: American Association of Cereal Chemists.

Osborne, B.G., T. Fearn and P.H. Hindle. 1993. Theory of near-infrared spectrometry. In: *Near Infrared Spectroscopy in Food Analysis.* Singapore: Longman Singapore Publishers.

Paliwal, J., S.J. Symons and C. Karunakaran. 2004. Insect species and infestation level determination in stored wheat using near-infrared spectroscopy. *Canadian Biosystems Engineering* 46: 7.17-7.24.

Pasikatan, M.C. and F.E. Dowell. 2004. High-speed NIR segregation of high- and low-protein single wheat seeds. *Cereal Chemistry* 81(1): 145-150.

Pearson, T.C., D.T. Wicklow, E.B. Maghirang, F. Xie and F.E. Dowell. 2001. Detecting aflatoxin in single corn kernels by using transmittance and reflectance spectroscopy. *Transactions of the ASAE* 44(5): 1247-1254.

Perez-Mendoza, J., J.E. Throne, F.E. Dowell and J.E. Baker. 2003. Detection of insect fragments in wheat flour by near-infrared spectroscopy. *Journal of Stored Products Research* 39: 305-312.

Prasad, L. and S.S. Iyengar. 1997. *Wavelet Analysis with Application to Image Processing*. CRC Press, Boca Raton, USA.

Roggo, Y., L. Duponchel, C. Ruckebusch and J.P. Huvenne. 2003. Statistical tests for comparison of quantitative and qualitative models developed with near infrared spectral data. *Journal of Molecular Structure* 654: 253-262.

Sinha, R.N. and F.L. Watters. 1985. *Insect Pests of Flour Mills, Grain Elevators, and Feed Mills and Their Control.* Ottawa, ON: Agriculture Canada.

Slaughter, D.C., K.H Norris and W.R. Hruschka. 1992. Quality analysis and classification of hard red winter wheat. *Cereal Chemistry* 69: 428-432.

Wang, D., F.E. Dowell and R.E. Lacey. 1999a. Single kernel color classification by using near-infrared reflectance spectra. *Cereal Chemistry* 76(1): 30-33.

Wang, D., F.E. Dowell and R.E. Lacey. 1999b. Single wheat kernel size effects on near-infrared reflectance spectra and colour classification. *Cereal Chemistry* 76(1): 34-37.

Wang, D., F.E. Dowell and D.S. Chung. 2001. Assessment of heat damaged wheat kernels using near-infrared spectroscopy. ASAE Paper No. 016006. St. Joseph, MI: ASAE.

Wang, D., F.E. Dowell and R. Dempster. 2002. Determining vitreous subclasses of hard red spring wheat using visible/near-infrared spectroscopy. *Cereal Chemistry* 79(3): 418-422.

Wang, D., F.E. Dowell, M.S. Ram and W.T. Schapaugh. 2004a. Classification of fungal-damaged soybean seeds using near-infrared spectroscopy. *International Journal of Food Properties* 7: 75-82.

Wang, W. and J. Paliwal. 2006. Generalization performance of artificial neural networks for near-infrared spectra analysis. *Biosystems Engineering* 94(1)7-18.

Wang, W., J. Paliwal and D.S. Jayas. 2004b. Determination of moisture content of ground wheat using near-infrared spectroscopy. *ASAE* Paper No. MB04-200. St. Joseph, MI: ASAE.

Wesley, I.J., O. Larroque, B.G. Osborne, N. Azudin, H. Allen and J.H. Skerritt. 2001. Measurement of gliadin and glutenin content of flour by NIR spectroscopy. *Journal of Cereal Science* 34: 125-133.

Williams, P.C. and D.C. Sobering. 1993. Comparison of commercial near-infrared transmittance and reflectance instruments for analysis of whole grains and seeds. *Journal of Near-Infrared Spectroscopy* 1: 25-32.