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Application of spectrometry in agricultural practices

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ABSTRACT

Human existence depends on receiving energy which is required for its body life and it is achieved by agriculture products and manufactured food. Supplying sufficient and qualified agricultural products require high-tech instrumentation and applying of appropriate tools which are adequate/reliable, fast, and non-destructive. Spectrometry, as a recent procedure of measurement and instrumentation, has found a venerable value in sciences, especially in agriculture and food industries. Field monitoring and quality control are the most important practices that are reported to be done by spectrometry methods. In this paper, some of these applications are reviewed. Finally, spectrometry, as a non-invasive, fast, and non-contact method of food monitoring, is suggested to agricultural specialists.

Keywords: non-invasive monitoring, quality control, spectrometry

INTRODUCTION

The world population increasing requires sufficient agricultural materials include food, feed, fiber, byproducts, and wasted materials in terms of quality and quantity. The agricultural material must be monitored during production to marketing. Therefore, high-tech methods of production are often required for supplying the increasingly demand for agricultural products.

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Abdel-Nour et al (2009) introduced visible/NIR spectroscopy as a powerful, fast and non-destructive technique that is increasingly used for measuring a large number of chemical and physical properties of agricultural products.

If a given sample is exposed with a band of frequencies, the sample's diffused reflectance is recorded using a spectrophotometer to form a reflectance spectrum which indicates the intensity of light collected as a function of wavelength (Sinfield et al, 2010). Visible/NIR spectroscopy is rapid, non-invasive, and could be used online, it is increasingly used for testing the quality of many agricultural products (Abdel-Nour et al, 2011).

Mass spectrometry can be considered as a powerful technique for identifying unknown materials. The technique is based upon the ion's motion, a charged particle, in an electric or magnetic field. Since the ratio of mass to charge (m/z) of the ion affects this motion and the charge of an electron is known, the mass to charge ratio is a measurement of an ion's mass. Typically, mass spectrometry researches focus on the formation of gas phase ions, the ions' chemistry, and applications of mass spectrometry (Van Bramer, 1998). The confinement of gaseous ions permits to study gas-phase ion chemistry and the clarification of ion structures by means of repeated stages of mass selection that is known as tandem mass spectrometry (March, 1997).

Proton transfer reaction mass spectrometry (PTR-MS), because of its high sensitivity and fast monitoring of volatile organic compounds, is applied to many fields of research and applications showing interesting performances (Biasioli et al, 2003).

In this paper, a review on some of applications of spectrometry in agricultural practices is reported.

1.1 Field monitoring

Since different groups of pigments absorb especial light wavelengths, spectroscopy can be used as a tool for quantification of phyto-pigment (Hilker et al, 2007). Non-destructive associated with rapid measurements of green biomass can be done in order to produce an index for defining the vegetation, such as the normalized difference vegetation index (NDVI), using a portable spectro-radiometer (Romano et al, 2011). The applications of multi-spectral images for crop production management have been studied since the late 1970s (Kang and Noguchi, 2011; Noh and Zhang, 2012).

Different visible and NIR spectral reflectance ranges due to changes in the chemical components of crop canopy motivate researchers to use it as a nondestructive way to sense the change happening inside the object (Li et al. 2012). One of the most accepted methods that is currently used to define crop canopy characteristics is spectral reflectance, which is measured by means of radiometers, spectrometers or digital cameras, and subsequent calculation of a vegetation index (Godwin, 2000; Gitelson et al., 2001; Miller et al., 2003; Scotford and Miller, 2004). But, Scotford and Miller (2004) introduced spectral reflectance techniques as the most popular method which is used to remotely sense both tiller density and leaf area index. However, technical restrictions had prevented the use of remote sensing for detection of pigment, the introduction of fine spectral resolution radiometers has provided opportunities to detect leaf-pigment concentrations at a range of scales from portable spectro-radiometers to airborne instruments (Hilker et al, 2007).

One of the most interesting subjects of precision agriculture is site-specific management of nitrogen and, therefore, accurate estimation of crops' nitrogen stress during side-dressing operations is essential for effectively site-specific management of nitrogen (Noh et al, 2006). This is demonstrated that the reflected light in specific visible, near- and middle-infrared regions of the electromagnetic spectrum is useful for detection of nutrient deficiencies, disease, weed, and insect infestations (Pydipati et al, 2006). Noh and Zhang (2012) investigated the shadow effect in the

image for developing a multi-spectral sensor to detect corn nitrogen deficiency based on crop canopy reflectance information from green (G), red (R), and NIR bands of light spectra.

On the other hand, using hyper-spectral imaging for nitrogen existence assessment has a great potential to overcome on many of the problems associated with estimations which are based on measurements of canopy reflectance with a low spatial resolution and it is now possible to obtain pure leaf estimates of the reflected light provided that the pixels have been pre-classified (Jorgensen, 2002).

“Phyto-pigments, consisting of carotenoids, chlorophylls, and anthocyanins, are organic compounds that are among the most important on earth, as they absorb solar radiation, and therefore are the ultimate source of energy for the terrestrial NIR spectroscopic determination of moisture concentrations that has already been performed in different scientific areas” (De Temmerman et al, 2007).

Since the spectral quality of reflections from affected trees is calibrated as the disease developments, spectra from trees in different health states were acquired and analyzed using a least squares technique to determine whether the health class could be assessed by a computer, then, the spectrum of a given tree was compared with a set of spectra representing trees of different health states. Computed solutions were in close agreement with the field observations (Pydipati et al, 2006).

Christy (2008) introduced an online spectrophotometer for in situ measurement of reflectance spectra and evaluating the potential of the system for making real-time prediction of various soil attributes using NIRS (Fig. 1).

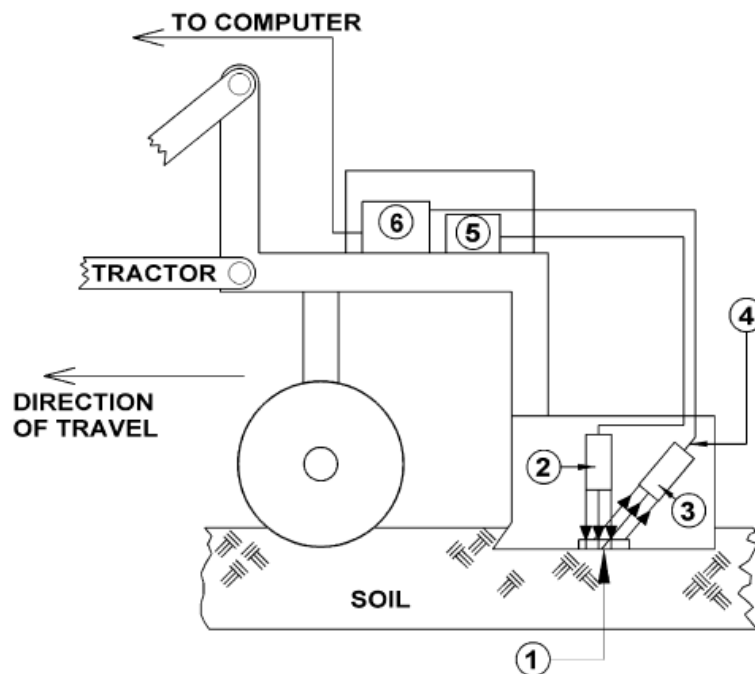


Fig. 1. The shank-based spectrophotometer used to obtain NIR reflectance spectra introduced by Christy (2008): (1) Sapphire window; (2) halogen lamp; (3) collection optic; (4) fiber optic; (5) spectrometer; (6) power supply.

1.2. Quality control

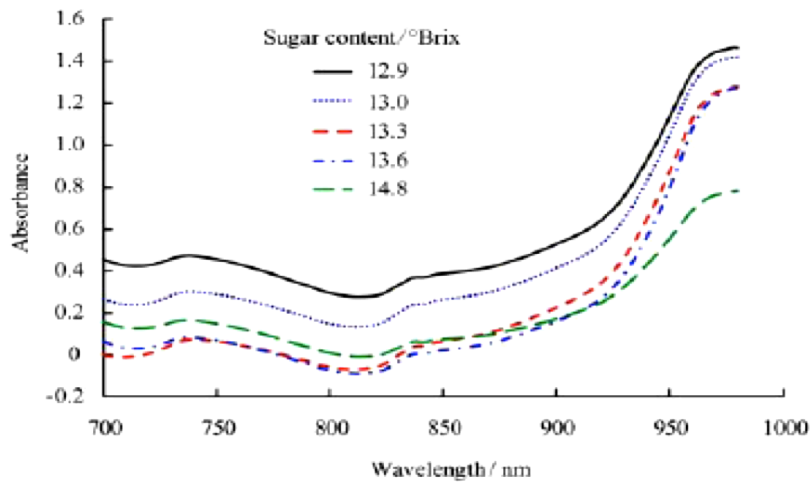
Since the mid-1970s, mass spectrometry has received attention for bacterial detection and differentiation caused by its capability when joined with chromatographic separation to identify particular compounds in complex mixtures. Fatty acids (Basile et al, 1995), proteins (Easterling et al, 1998) and complex lipids (Helen et al, 2004) have been used in distinguishing bacterial samples (Zhang et al, 2011).

Controls on aroma are being done by human experts yet. The men test and evaluate the wine by perceiving the volatile compounds in the headspace and therefore, Lasekan and Otto (2009) suggested an automatic technique, i.e. proton transfer reaction-mass spectrometry, which can reproduce the sensitivity of the human nose is highly important.

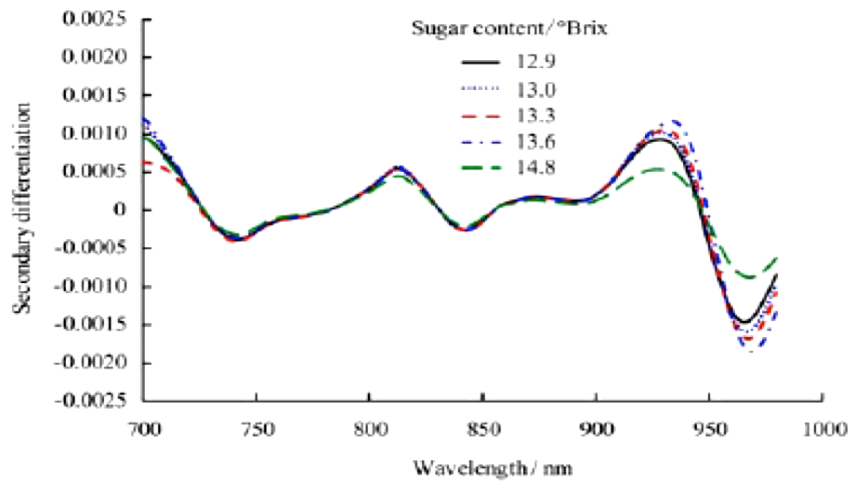
A comprehensive analysis of the coffee headspace brew using proton-transfer-reaction mass-spectrometry was carried out by Yeretian et al (2003). They introduced a set of methods that linked mass spectral peaks, as observed in PTR-MS, to chemical compounds in the headspace of coffee and by combining all this information, an experimental assignment and rough quantification of liquid coffee headspace was presented by them.

Ruth et al (2003) compared three methods included systems with olfactometry detection, flame ionization detection, and mass spectrometry; for the analysis of the aroma of rehydrated diced red bell peppers. They understood that the proportions of the odour active compounds were not significantly different for mass spectrometry, flame ionization detection, and PTR-MS.

Mayr et al (2003) monitored the air exhaled through the nose, by a PTR-MS, and the time intensity profiles of a series of volatiles in order to analysis of volatiles released in the mouth during eating of ripe and unripe banana. Lee et al (2007) used matrix assisted laser desorption/ionization time of flight mass spectrometry to analyze the in vitro glycation of peptides/proteins. Yamakawa et al (2012) developed a system for quality monitoring of citrus fruit. .it is consisted of a light detection , ranging (LIDAR) and visible-near infrared spectroscopy sensors which was installed on a sloping conveyer for real-time fruit size and total soluble solids (TSS) measurement, respectively (Fig. 2).



a. Raw absorbance for citrus fruits with different levels of TSS



b. Resulting secondary differences of spectral signatures

Fig. 2. Typical raw absorbance and resulting secondary differences of spectral signatures for citrus fruits with different levels of TSS (Yamakawa et al, 2012).

Suphamitmongkol et al (2013) achieved an accurate classification of Thai oranges by using of near infrared spectroscopy (NIRS) for non-destructive discriminating Thai orange varieties (Fig. 3).

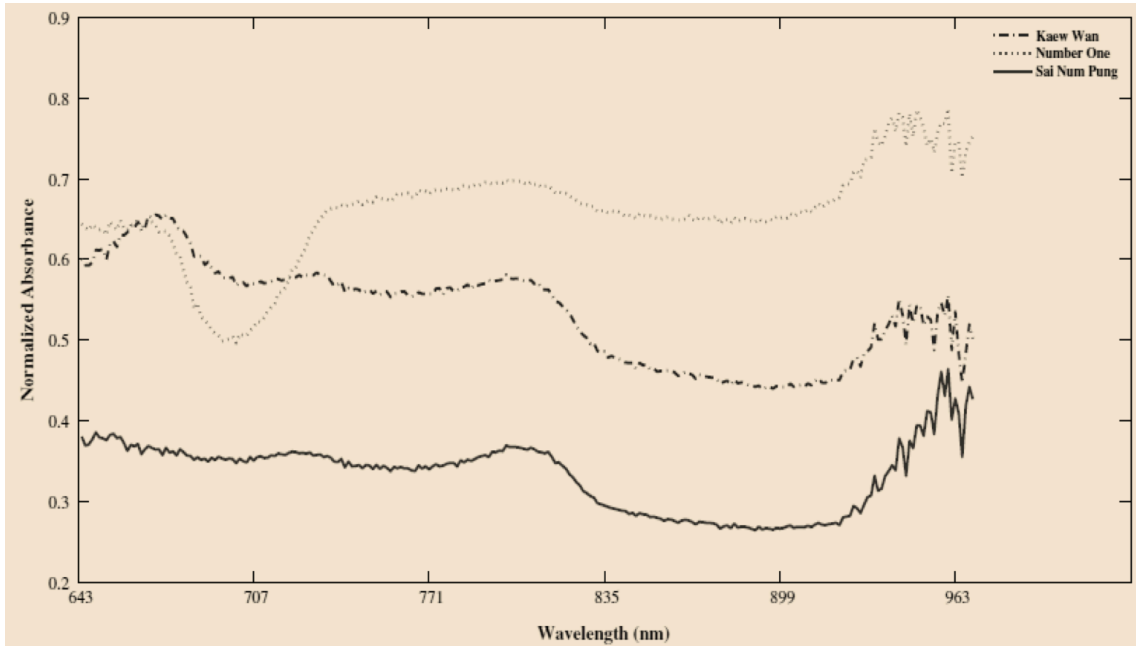


Fig. 3. The average NIR absorbance of the three orange varieties at different spectra (identified by wavelength) (Suphamitmongkol et al, 2013).

The NIR reflectance spectroscopy is also proposed for in-line determination of moisture concentrations in semolina pasta without delay after the extrusion process by Hilker et al (2012).

DISCUSSIONS

According to the reviewed literatures, spectrometry has a vast domain of applications in agricultural practices. Field monitoring and quality control of agricultural crops require adequate, fast, non-contact and low cost methods. Therefore, intelligent instrumentation would be an appropriate alternative for agricultural industries.

Visible and NIR ranges are the most spectra that the researchers have focused on for agricultural applications. Infect detection, greenness defining, mass estimation, moisture discrimination, chemical compounds analysis, and many other measurements can be done by spectrometry.

Considering spectroscopy, as a modern technique, would contribute more in progress of the procedures. Therefore, as an alternative, it is suggested to researchers to pay more attentions to the associated costs and the policies to decline the costs associate with the conventional methods of doing the agricultural practices.

CONCLUSION

This short review illustrated spectrometry methods are important practices as a non-invasive and fast technique for field monitoring and quality control in agriculture and food industries. Visible and NIR reflectance were considered as the most spectral ranges that researchers have focused for agricultural applications. Infect detection, greenness defining, mass estimation, moisture discrimination, chemical compounds analysis, and many other measurements can be done by spectrometry.

REFERENCES

- Abdel-Nour, N., Ngadi, M., Prasher, M., Karimi, Y., 2009. Combined maximum R^2 and partial least square wavelengths selection and analysis of spectroscopic data. *International Journal of poultry science*, 8(2),170-178.
- Abdel-Nour, N., Ngadi, M., Prasher, M., Karimi, Y., 2011. Prediction of egg freshness and albumen quality using visible/near infrared spectroscopy. *Food Bioprocess Technol*, 4:731–736.
- Basile, F., K.J. Voorhees and T.L. Hadfield. 1995. Microorganism gram-type differentiation based on pyrolysis-mass spectrometry of bacterial fatty acid methyl ester extracts, *Appl. Environ. Microbiol*, 61:1534–1539.
- Christy, C.D. 2008. Real-time measurement of soil attributes using on-the-go near infrared reflectance spectroscopy. *Computers and Electronics in Agriculture*, 61:10–19.
- De Temmerman, J., W. Saeys, B. Nicolai and H. Ramon. 2007. Near infrared reflectance spectroscopy as a tool for the in-line determination of the moisture concentration in extruded semolina pasta. *Biosystems Engineering*, 97:313-321.
- Easterling, M.L., C.M. Colangelo, R.A. Scott and I.J. Amster. 1998. Monitoring protein expression in whole bacterial cells with MALDI time-of-flight mass spectrometry, *Analyt. Chem*, 70:2704–2709.
- Gitelson, A.A., M.N. Merzlyak, Y. Zur, R Stark and U. Gritz, 2001. Non-destructive and remote sensing techniques for estimation of vegetation status. In: *Proceedings of the 3rd European Conference on Precision Agriculture ECPA* (Blackmore S; Grenier G, eds), pp 205–210, Montpellier, France.
- Godwin, R.J. 2000. Precision farming—a multi disciplinary approach for cereal production. *Institution of Agricultural Engineers, Landwards*, 55(2), 4–9.
- Helen, F.S., E.S. Roger, S. Kristin, E. Marcus and H. Kai-Uwe. 2004. Intact polar membrane lipids in prokaryotes and sediments deciphered by high-performance liquid chromatography/electrospray ionization multistage mass spectrometry – new biomarkers for biogeochemistry.
- Hilker, T., N.C. Coops, Z. Nestic, M.A. Wulder and A.T. Black. 2007. Instrumentation and approach for unattended year round tower based measurements of spectral reflectance. *Computers and Electronics in Agriculture*, 56:72–84.
- Jorgensen, R.N. 2002. Study on Line Imaging Spectroscopy as a Tool for Nitrogen Diagnostics in Precision Farming. PhD Thesis. The Royal Veterinary and Agricultural University, Copenhagen, Denmark
- Kang, T.H., Noguchi, N., 2011. Estimation of the potato growth information using multi-spectral image sensor. *Journal of Biosystems Engineering* 36 (3), 180–186 (In Korean).
- Lasekan, O. and S. Otto. 2009. In vivo analysis of palm wine (*Elaeis guineensis*) volatile organic compounds (VOCs) by proton transfer reaction-mass spectrometry. *International Journal of Mass Spectrometry*, 282:45–49.

- Lee, B.S., S. Krishnanchettiar, S.S. Lateef and S. Gupta. 2007. Analyses of the in vitro non-enzymatic glycation of peptides/proteins by matrix-assisted laser desorption/ionization mass spectrometry. *International Journal of Mass Spectrometry*, 260:67–74.
- Li, X., W.S. Lee, M. Li, R. Ehsani, A.R. Mishra, C. Yang and R.L. Mangan. 2012. Spectral difference analysis and airborne imaging classification for citrus greening infected trees. *Computers and Electronics in Agriculture*, 83:32–46.
- March, R. 1997. An introduction to quadrupole ion trap mass spectrometry. *Journal of Mass Spectrometry*. 32:351-369.
- Mayr, D., T. Mark, W. Lindinger, H. Brevard and C. Yeretizian. 2003. Breath-by-breath analysis of banana aroma by proton transfer reaction mass spectrometry. *International Journal of Mass Spectrometry*, 223–224:743–756.
- Noh, H. and Q. Zhang. 2012. Shadow effect on multi-spectral image for detection of nitrogen deficiency in corn. *Computers and Electronics in Agriculture*, 83:52–57.
- Noh, H., Q. Zhang, B. Shin, S. Han and L. Feng, 2006. A neural network model of maize crop nitrogen stress assessment for a multi-spectral imaging sensor. *Biosystems Engineering*, 94(4):477–485.
- Pydidpati, R., T.F. Burks and W.S. Lee. 2006. Identification of citrus disease using color texture features and discriminant analysis. *Computers and Electronics in Agriculture*, 52:49–59.
- Romano, G., S. Zia, W. Spreer, C. Sanchez, J. Cairns, J.L. Araus and J. Muller. 2011. Use of thermography for high throughput phenotyping of tropical maize adaptation in water stress. *Computers and Electronics in Agriculture*, 79:67–74.
- Ruth, S.V., E. Boscaini, D. Mayr, J. Pugh and M. Posthumus. 2003. Evaluation of three gas chromatography and two direct mass spectrometry techniques for aroma analysis of dried red bell peppers. *International Journal of Mass Spectrometry*, 223–224:55–65.
- Scotford, I.M. and P.C.H. Miller. 2004. Estimating tiller density and leaf area index of winter wheat using spectral reflectance and ultrasonic sensing techniques. *Biosystems Engineering*, 89(4):395–408.
- Sinfield, J.V., D. Fagerman and O. Colic. 2010. Evaluation of sensing technologies for on-the-go detection of macro-nutrients in cultivated soils. *Computers and Electronics in Agriculture*, 70:1–18.
- Suphamitmongkol, W., G. Nie, R. Liu, S. Kasemsumran and Y. Shi. 2013. An alternative approach for the classification of orange varieties based on near infrared spectroscopy. *Computers and Electronics in Agriculture*, 91:87–93.
- Van Bramer, S.E. 1998. An introduction to mass spectrometry. Widener University. Available at: <http://science.widener.edu/~svanbram>.
- Yamakawa, M, L.R. Khot, R. Ehsani and N. Kondo. 2012. Real-time nondestructive citrus fruit quality monitoring system: development and laboratory testing. *Agric Eng Int: CIGR Journal*, 14(3):117-124.
- Zhang, J.I., N. Talaty, A.B. Costa, Y. Xia, W.A. Tao, R. Bell, J.H. Callahan and R.G. Cooks. 2011. Rapid direct lipid profiling of bacteria using desorption electrospray ionization mass spectrometry. *International Journal of Mass Spectrometry*, 301:37–44.