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Uncertainty factors of measuring protocol in laboratory spectroscopy

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Abstract

There are many research institutes and official organizations that use spectroscopic analysis methods in basic studies or even offer its service on the area of remote sensing. Depending on the aim of the study there are many types of desktop spectrum analysers and portable (dual-purpose) spectroradiometers offering various precision and reliability. The lack of a real standard measuring environment and measuring protocol really raises difficulties to provide repeatable measurements or even to utilize, reach the maximal precision of a certain device, especially in case of portable spectroradiometers under laboratory conditions. The situation can be even worse when analysing raw samples. In this study we are introducing a basic study which aims to reach the maximal precision offered by an ASD FieldSpec 3 MAX spectroradiomer to identify the optical characteristics of Fusarium infected wheat samples to facilitate an effective non-destructive separation method in agricultural production.

Keywords: Spectroscopy, Fusarium, postharvest selection

1 Introduction

As the trend of healthy alimentation grows the production and marketing of whole grain products are rises. More and more people pay attention to change to these products. In accordance with the spreading of another decisive tendency, which might be called bio-trend-line, the demand toward ecologically produced whole grain products is rising. Due to the bran content of such foods the risk of health problems caused by various fungal diseases and toxins increases. This must be considered as important hazard factor. The strict regulation of chemical protection makes difficult to guarantee the fungal disease-free production of cereals so decisive quantity of the grain cannot be qualified as sound raw material for further processing. Beside the resistant or tolerant varieties and the favourable climate conditions one solution is the postharvest selection, the separation of sound and infected kernels.
The traditional laboratory technologies are rather time, cost and labour-intensive methods and not capable of performing high speed selection which – considering the usual harvested quantity - is necessary to reach a desirable effectiveness. A possible solution for the separation is the remote sensing. One of these non-destructive analytical technologies is the spectroscopy, which studies the interaction between electromagnetic radiation and matter. It provides opportunity to obtain quantitative relationships between the environmental and physiological parameters of organic or non-organic samples, plant parts, soil quality parameters and the features of reflectance spectra (Erdélyi et al. 2009, Balla et al. 2011, Máthé et al. 2010, Tolner 2011, Tarnawa et al. 2011). Characteristic wavelengths can indicate changes in moisture content and other relevant parameters (Kaszab et al. 2008, Milics et al. 2010). Based on sci-

entific references spectral evaluations were proved to be useful in detecting and diagnose certain fungal diseases (Neményi 2013, Virág and Szőke 2011). For sample analysis an ASD FieldSpec 3 Max portable spectroradiometer was used under laboratory conditions to extend the range of the detectable visible light (Lágymányosi and Szabó 2009, Lágymányosi and Szabó 2011) to NIR (near infrared) and the SWIR (shortwave infrared) region. Despite the available technical background, thermal features have were not tested (Kátai et al. 2013).

2 Materials and methods

Laboratory tests we carried out in a light-isolated cabinet. Data acquisition was made with ProLamp (Figure 4.) illumination from a distance of 70 cm.

Figure: 4 ProLamp

In this study we have evaluated the stability of results – at ProLamp - received by putting back the same sample. Results showed rather high variation in the spectra Figure 5 and Figure 6.

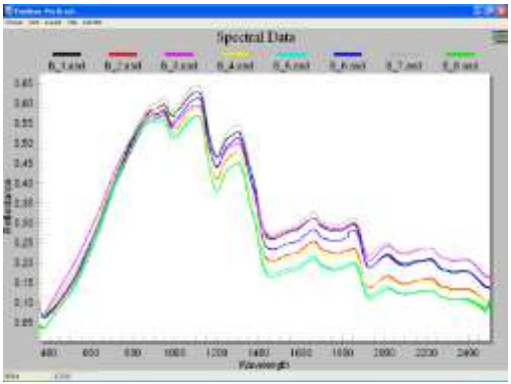

Figure 5 : Reflectabce spectra of the same wheat sample

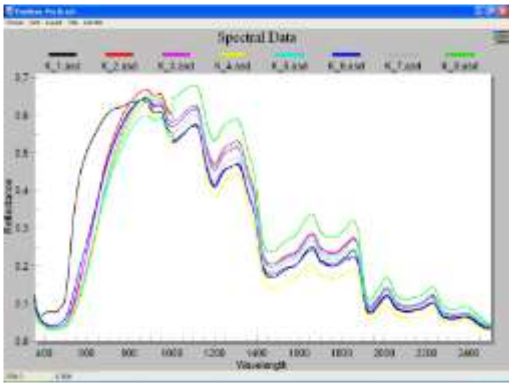

Figure 6 : Reflectance spectra of the same maize sample

The original ProLamp provided a simply one-sided and only partially homogenous illumination. Upon the preliminary results the surficial changes in the micro-relief of the sample affects the recorded spectra. This affect had been tested by rotating the samples by 0°, 90°, 180°, 270°. The change in light/shadow balance definitely increases the uncertainty. These factors have been risen a need for designing a new illumination. The following demands have been laid toward the new illumination: providing with 350-2500 nm range electromagnetic radiation, well-focused, homogenous, adjustable illumination angle.

Focus, homogeneity and spectral distribution were examined. Results are illustrated with figures Figure 7.

Figure 7: The inhomogeneous projection of the Pro Lamp

According to the our tests, a 12 V 55W halogen illuminant and a 84 mm in diameter housing were chosen as a light source. A special frame was designed and manufactured to hold 8 pieces of lamps. This frame was installed inside the light isolated laboratory cabinet (Figure 8). Homogeneous light was focused directly to the sample plate (Figure 9).

Figure 8: Multidirectional illumination

Figure 9: Homogeneous projection

3 Results

After developing the above described illumination system we repeated the measurements with the same maize and wheat samples, with the same number of repetition. The differences between the spectra, which were recorded from the same sample, but from various angles, reduced significantly. The reduction of the calculated standard deviation is illustrated with Figure 10. and Figure 11.

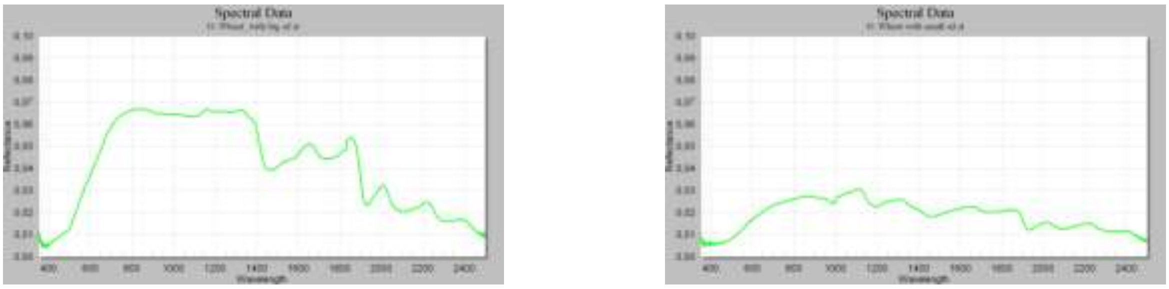

Figure 10: The reduction of standard deviation in case of wheat. Measurement with new illumination - on the right

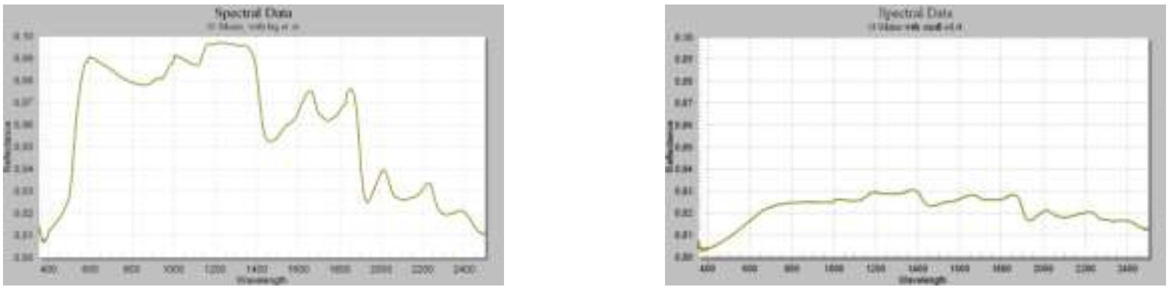

Figure 11: The reduction of standard deviation in case of maize. Measurement with new illumination - on the right

4 Conclusions

A well-focused, homogenous and multidirectional illumination was developed to significantly increase the reliability of the spectral measurements in laboratory. Normalization techniques can further increase the reliability. This facilitates to detect and identify even smaller differences, characteristics referring to existed infection of kernels.

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