WHEAT AND TRITICALE WHOLE GRAIN SINGLE KERNEL HYPERSPECTRAL IMAGING: RESOLVING A COMPLEX DATA SET

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ABSTRACT

Near infrared (900-2500nm) hyperspectral imaging (HySpex SWIR 640) was used as the primary analytical technique for quantification of single kernel protein and moisture content and kernel hardness for wheat and triticale whole grain kernels. Wheat (*Triticum aestivum*) is one of the most important cereal crops grown globally. Triticale (× *Triticosecale* sp. Wittmack ex A. Camus 1927) is an important cereal crop for feed and fodder production and is also emerging as an alternative cereal for human consumption. Both these cereals are grown and produced in a diverse climatic environment and they vary with regards to their physicochemical properties. Quantitative techniques for determining protein and moisture content and kernel hardness are of importance for grading of the grains. The use of non-invasive and rapid techniques such as near-infrared hyperspectral imaging (NIR-HSI) show potential for quantification of these quality parameters. This study aimed to investigate the use of NIR-HSI with partial least squares regression (PLS-R) analysis using the SIMPLS and comparatively the RSIMPLS algorithms for wheat and single kernel image approaches.

The study considered South African wheat and triticale samples produced in three Western Cape localities, i.e. Napier, Tygerhoek and Vredenburg, comprising 180 wheat and 177 triticale samples. Of these, 39 kernels per sample were used for single kernel protein and moisture content and kernel hardness prediction, resulting in data sets with a total of 7020 wheat, 6903 triticale and 13923 combined single kernel images.

NIR (1100-2100 nm) hyperspectral images were acquired and the spectral data obtained for each pixel were averaged for each kernel. PLS-R was used to develop quantitative prediction models. Principal component analysis (PCA) was performed for the combined wheat and triticale data set – no separation was noted between the two sets of data (PC1 vs. PC2. Bulk sample protein, moisture content and kernel hardness models were first evaluated which showed favourable prediction accuracy, comparable to conventional NIR spectroscopy studies performed on wheat and triticale. The combined dataset for protein and moisture content and hardness prediction had RMSEP-values of 0.41%, 0.49% and 8.66, respectively.

Single kernel analysis involved two main quantitative data analysis methods (PLS-R (SIMPLS) and Robust-PLS (RSIMPLS), which were tested with an independent test set. The results being favourable for the conventional PLS-R method when only the validation set RMSEP (protein content: 0.37-0.84%, moisture content: 0.23-0.57% and kernel hardness: 1.74-3.64) was considered. The independent test set for protein content prediction achieved better results with the Robust-PLS (RMSEP protein content: 1.95-2.37%) method, proving that the method did indeed have an effect on making the calibration models more robust.

Spectral imaging as an analytical technique showed that it is capable of accurately quantifying protein and moisture content and kernel hardness of whole single kernels. With good robust models being optimal for quantification of these properties. The technique shows good potential for further study and to build onto the current data sets for models (protein, moisture and kernel hardness) that had R^2-values higher than 0.75 (RPD > 2) (Fig. 1) by adding samples from further seasons and localities to increase variance.

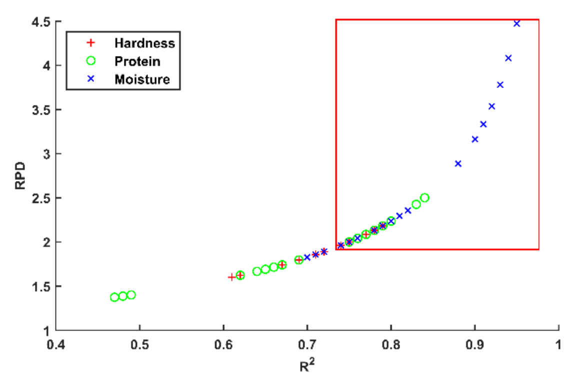

Figure 1 RPD vs. R^2-values for single kernel protein and moisture content prediction and kernel hardness models. Models with an RPD > 2 (R^2 > 0.75) (outlined) are suitable for further development.