Application Note 50: Cropscan 2000B Prediction of Malting Barley.

Introduction

The analysis of barley for protein and moisture content is important for malting. The Cropscan 2000B Whole Grain NIR Analyser was tested for the measurement of protein and moisture using 70 Australian barley samples using a calibration developed from malting grade barley samples collected throughout Australia.

Description

381 spectra of Australian malting grade barley samples were collected using several Cropscan 2000B Whole Grain NIR Analysers. The spectra were combined to form a calibration set. The reference data for half the samples were from Dumas method for Nitrogen, oven drying for moisture, and the other half were taken from a Foss Infratec™ 1241. The 381 spectra were collected using a 15mm pathlength sample cell and scanned from 720-1100nm. 9 scans of each sample were collected in the Cropscan 2000B and then averaged in Microsoft Excel to form 1 spectra per sample. The 381 spectra were imported into NTAS(NIR Technology Australia Software) to perform a Partial Least Squares (PLS) calibration.

A completely separate sample set of 70 South Australian malting grade barley samples were used as a test set for the above calibration. Ten scans of each sample were collected and averaged to give a single prediction result for protein(as is) and moisture. An outlier detection method, Z Scores, were used to reject any of the 10 scans with a Z Score greater than 1.5. Out of this prediction set, 16 samples were scanned twice in order to determine the repeatability of the Cropscan 2000B.

Results

Calibration Data:

The results of the PLS calibration for protein and moisture are shown below.

	Number of spectra (n)	Range (%)	Number of Principal Components (PC's)	Correlation (R)	Standard Error of Calibration (SEC)
Barley Calibration					
Protein	381	7 – 14.3	15	0.92	0.39
Moisture	72*	8 - 12	5	0.99	0.17

* Of the 381 barley samples, only 72 had recent moisture analyses. As such, the moisture calibration was developed using only 72 spectra.

A graphical representation of the calibration data is presented below.

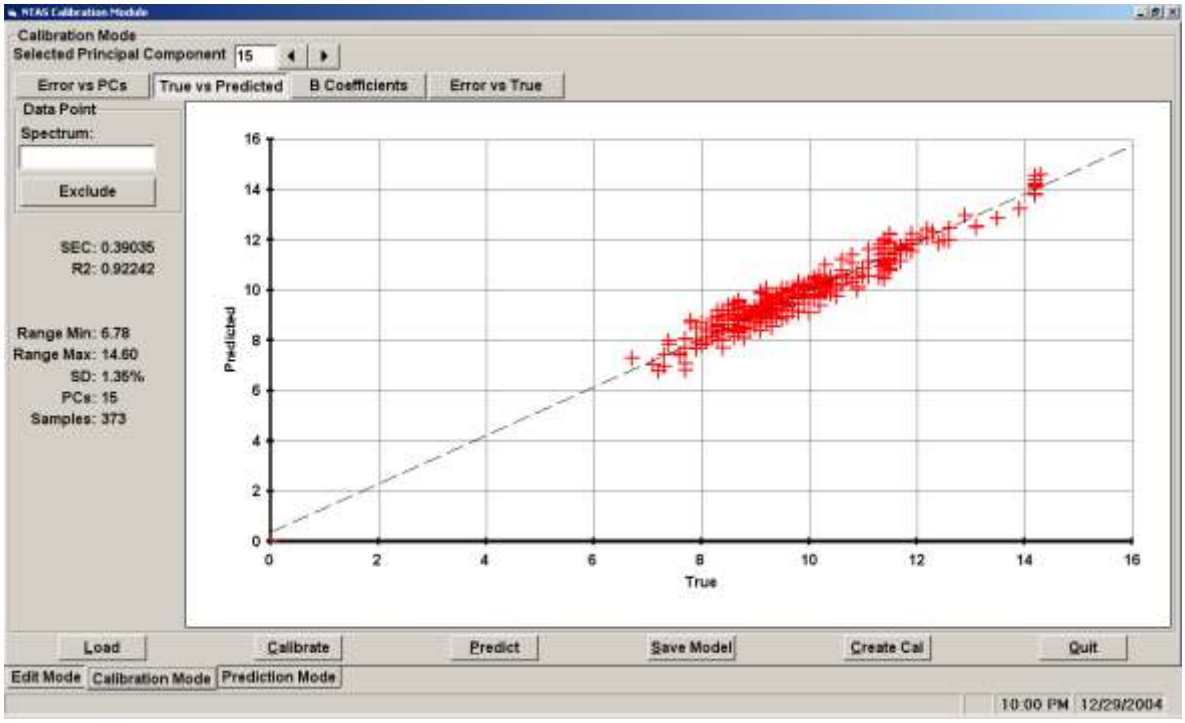

Figure 1. Calibration Plot, Protein

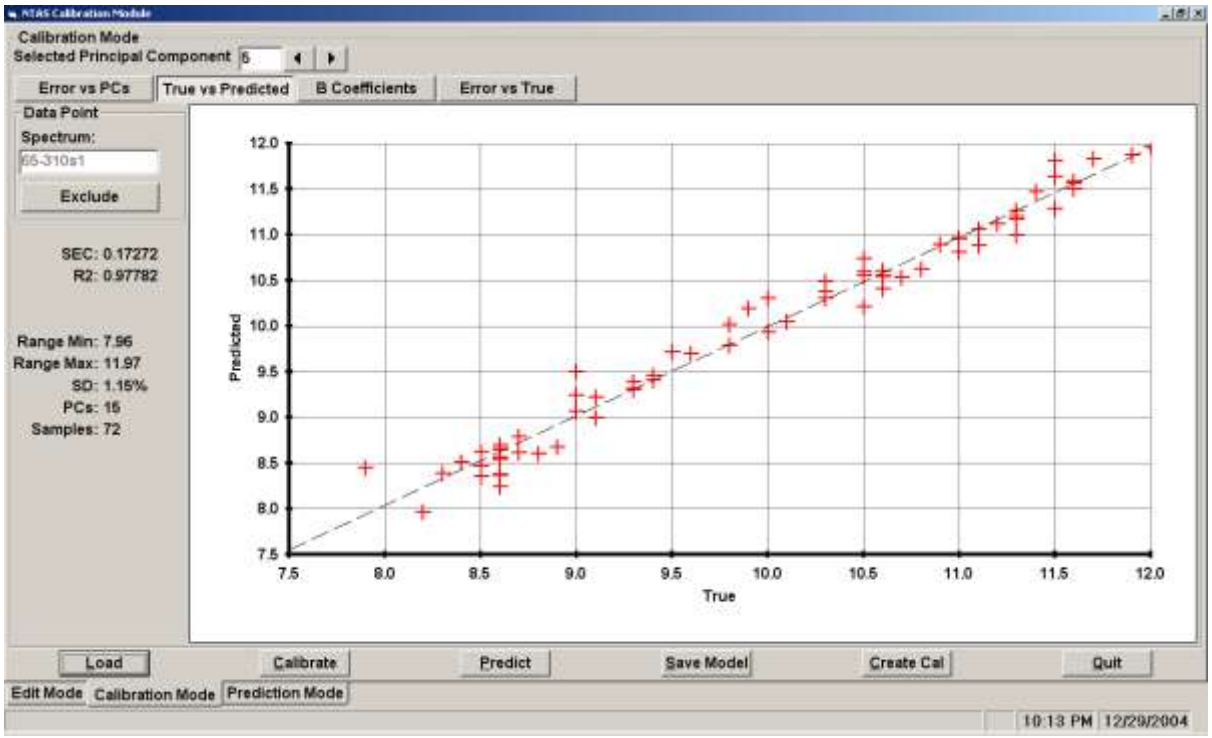

Figure 2. Calibration Plot, Moisture.

Prediction Data:

The results of predicting the 70 samples are presented below;

	Number of Spectra (n)	Range (%)	Number of Principal Components (PC's)	Correlation (R)	Standard Error of Prediction (SEC)
Barley Prediction					
Protein	99	8.5 - 12	12	0.85	0.32
Moisture	99	8 - 12	8	0.96	0.16

The graphical representations of these data are presented below:

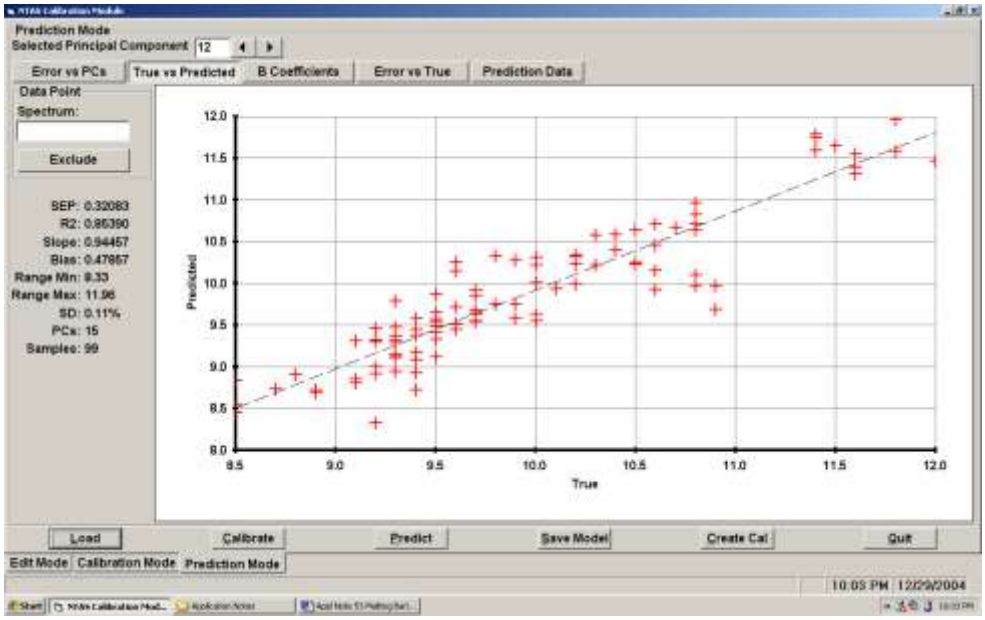

Figure 3. Prediction Plot, Protein

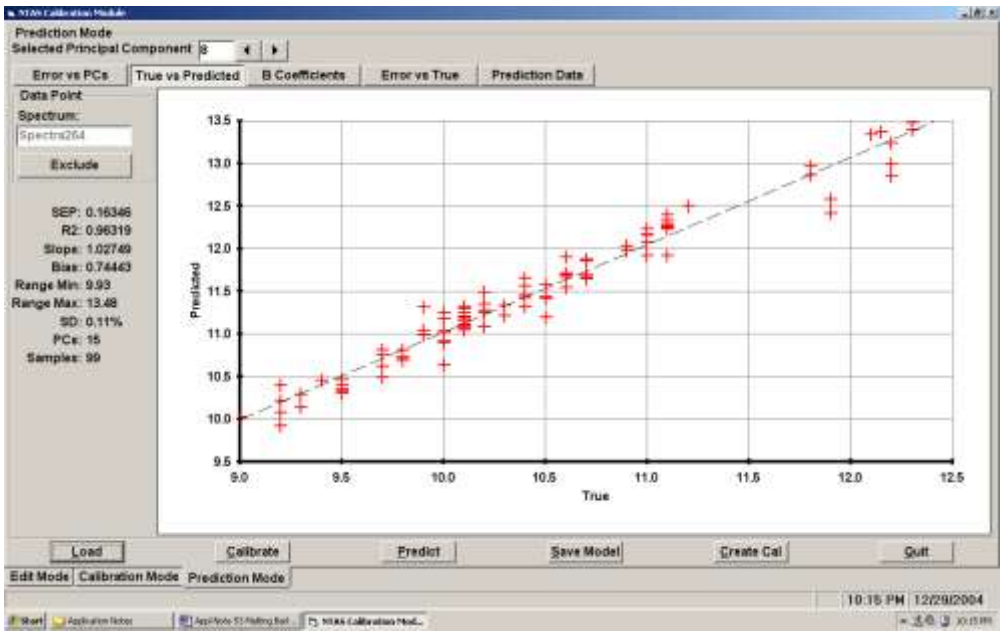

Figure 4. Prediction Plot, Moisture.

Repeatability:

	Number of Spectra (n)	Range (%)	Number of Principal Components (PC's)	Standard Deviation of Difference	
Barley Repeatability					
Protein	16	8.5 - 12	12	0.24	
Moisture	16	8 - 12	8	0.13	

Discussion:

The development of calibrations for protein and moisture in barley is a more complex task than for wheat. Varietal differences in barley, along with regional growing conditions, tends to produce barley with a greater variation in NIR spectra. It has been noted that the hull of the barley seed can become detached from the endosperm and thereby affect the NIR spectra. As well, barley straw, eg, horns, is far more prevalent in barley samples than in wheat samples. Since NIR analysers only measure the amount of light that passes through a sample of grain, then the detached hull, presence of straw and the considerable range in seed size of barley samples, then it is to be expected that barley calibrations will show larger errors than wheat calibrations.

The calibration for protein in barley shown in this report, is considered to exhibit too large an Standard Error of Calibration (SEC) There are two reasons for this high SEC; 1) the 381 samples were sourced from across Australia and represent a broad range of varieties and growing conditions, and 2) the reference data comes from several sources, ie, different laboratories for the Dumas and oven drying methods and from 2 Foss Infratec 1241 analysers. However calibration statistics only show the variation that exists between the reference data and the NIR spectra. The prediction data is a far better determinant of the robustness of the calibration. Since the prediction data shows significantly improvement over the calibration data, the evaluation of the system is based on the prediction data. To illustrate the issue of calibration data being misleading, the 381 samples were reduced to the same 72 samples used for the moisture calibration and a second protein calibration developed. Figure 7 shows the calibration plot.

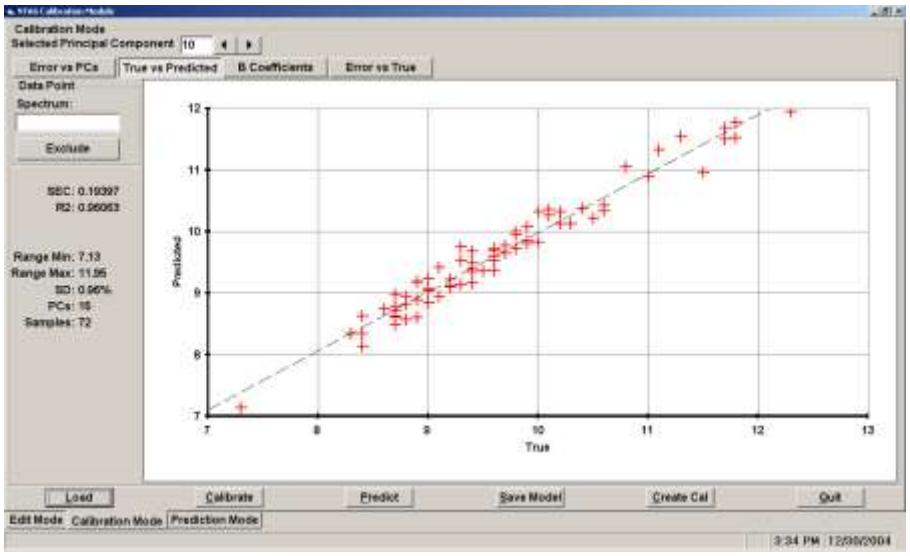

Figure 7. Calibration Plot – Protein, 72 samples only.

Using this calibration for prediction against the 70 samples in the prediction set, produces a slightly better SEP, ie, 0.3% vs 0.32% for the original calibration, see figure 8. However this new calibration does not predict the other barley samples well.

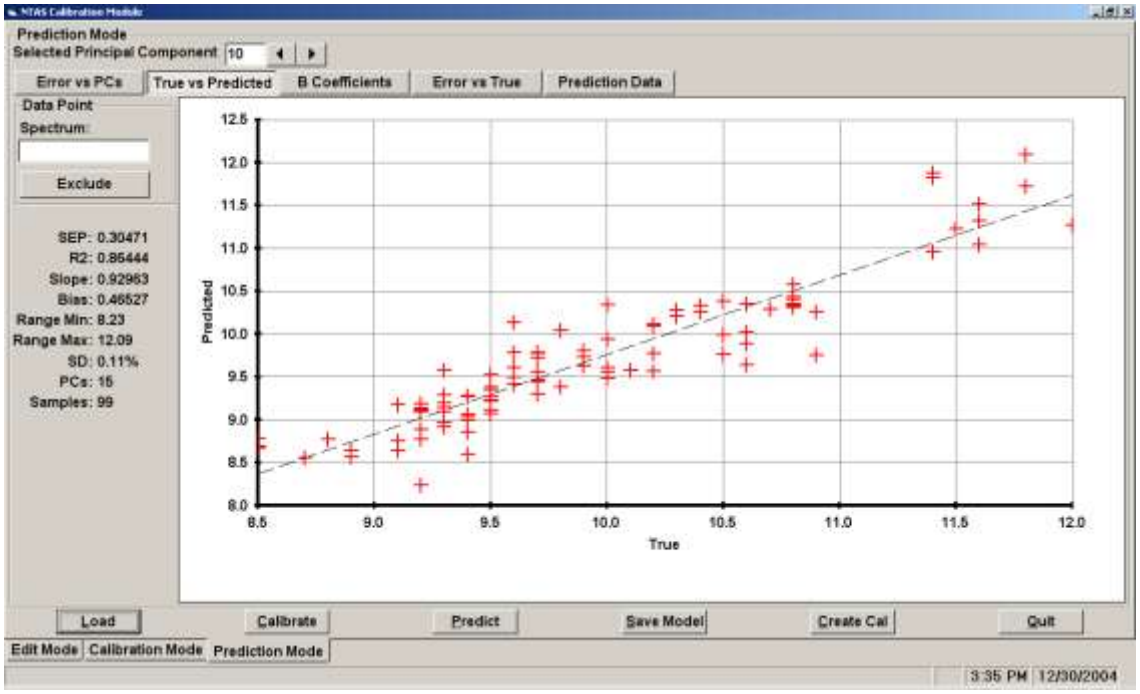

Figure 8. Prediction Plot – Protein, 70 samples.

The calibration and prediction for moisture in barley is very good. The SEC of 0.17% and the SEP of 0.16%, shows that the calibration holds up well. However this calibration is based on too few samples and would be improved if there were 300-400 spectra used.

Conclusion:

The Cropscan 2000B has been designed to measure protein and moisture in grains and oil and moisture in oil seeds. The data presented in this report illustrates the accuracy and repeatability of the instrument. It should be noted that Australian malting grade barley samples are generally very white and clean. Other barley samples such as feed grades, do not calibrate as well as malting grade barley. And many international varieties also do not calibrate well due to greater variations in colour, size and condition.

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