On-Line Roasted Coffee Quality Control Using NIR Spectroscopy

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SUMMARY

Roasting is a key stage in the production of high quality coffee and this step must be controlled and reproducible to meet consumer expectations. The coffee organoleptic and physico-chemical characteristics have to be evaluated close to the process to assure fine monitoring of the roaster conditions. In 2006, a study was done in collaboration with Kraft Foods to evaluate the feasibility of using Near Infrared Spectroscopy (NIRS) to control coffee quality at discharge from the roasters. The study focused on moisture content determination using a NirOnline Xtwo spectrometer (Nir-Online, Walldorf, Germany). For this study, 284 samples of Arabica and Robusta coffees were roasted under industrial conditions and at the laboratory, and then remoistened to obtain a range of moisture content from 1% to 6%. Coffee beans were analysed in continuous mode using the Xtwo spectrometer and in a static mode using a FOSS 6500 laboratory spectrometer (FOSS, Port Matilda, USA). Calibrations were developed using partial least squares regression to predict moisture content of the coffee batches for each instrument. The performances in terms of accuracy and robustness of each calibration for continuous mode and for static mode were compared. The standard errors of prediction (SEP) of each calibration were similar, 0.18% for the FOSS spectrometer and 0.19% for the NIR-Online spectrometer. These levels of accuracy were very close to those obtained with the FOSS instrument for ground roasted coffee and to the standard error of laboratory reference method (SEL = 0.1%). This study confirms the possibility of at-line monitoring of the roasting step using near infrared spectroscopy. The next step will be the implementation of NIRS technology in the coffee roasting chain to automate and control the roaster parameters.

INTRODUCTION

This study, carried out in 2006 in collaboration with Kraft Food (Lavérune, France) focused on continuous and rapid (about 30 ms) determination of moisture content using a NIR spectrometer (model Xtwo, Nir-Online, Walldorf, Germany) in order to monitor the roasting process. Predictive models using partial least squares regression (PLSR) were developed that gave accurate estimations (± 0.4%) of final roasted coffee moisture content.

EXPERIMENTAL PROCEDURE

For this study, 284 samples of Arabica and Robusta coffees from different geographical origins, were roasted under industrial conditions (continuously and in batches) and at the laboratory using a Probat PRE 1Z (Belgium) roaster (slow roasting) and a Neuhaus Neotec RFB (Germany) roaster (fluidized-bed fast roasting). Samples were remoistened in a controlled cabinet (FIRLABO, SP-BVEHF, Meysieu, France) at 60% RH and 28 °C, to obtain a range of moisture content from 1 % to 6 %. Coffee beans were analysed in continuous mode using the Xtwo spectrometer and in a static mode using a Foss 6500 (FOSS, Port Matilda, USA) laboratory spectrometer.
A validation set of 35 samples: 22 with final roasting moisture content and 13 remoistened samples in order to cover the total range, was analysed on both instruments. Moisture content was determined by gravimetry at 103 °C for 16 hours using a Chopin oven.

**Near Infrared Spectroscopy**

X-Two is a compact and rugged NIR spectrophotometer unit equipped with automatic internal referencing and a dual light source. Diode array detectors are used to provide simultaneously measured data across the complete spectral range (950 nm to 1750 nm) for one kilogram coffee bean samples. The Foss 6500 spectrometer is a grating-monochromator type and was equipped with a transport module and rectangular cell. Diffuse reflectance spectra (400 nm to 2500 nm) were recorded using about 150 g of coffee beans. The spectra were mathematically transformed using WINISI v.1.5 software (Infrasoft International, Port Matilda, USA): the second derivatives of standard normal variate and detrend corrected and smoothed spectra were computed.

Moisture calibration was performed using partial least squares regression (PLSR). Calibration statistics used to evaluate model performance included standard error of calibration (SEC), coefficient of determination (R²), standard error of cross-validation (SECV) and standard error of prediction (SEP). The RPD ratio (RPD=SD/SEP) was also used to evaluate the performance of each equation. The Student test (t) was used to identify t-outlier samples.

**RESULTS**

The 284 calibration samples analyzed had an average moisture content of 3.99% with a maximum of 6.00% and a minimum of 1.95%. The average moisture content for the 35 validation samples was 4.36%, with a distribution covering the whole range of moisture content, but concentrated in the range 3.5-6% (Figure 1).

![Figure 1. Moisture content distribution for calibration and validation samples.](image)

The average NIR spectra for the NIR-online and Foss instruments (Figure 2) showed similar profiles, with a slight shift in absorbance band peaks, almost certainly due to differences in operating software wavelength codifications. These plots allowed the 3 principal absorption bands due to H-OH vibrations (1100 nm, 1340 nm and 1900 nm) to be identified. Because of its reduced spectral range (950 nm -1750 nm) the higher band (1900 nm, first overtone of H-OH) was not accessible to the NIR-Online instrument.
Figure 2. Average spectra of roasted beans measured on the NIR-Online and FOSS spectrometers.

The plot of the standard deviation of absorbance value calculated for each wavelength for NIR-Online spectra showed a maximum value at 1340 nm, corresponding to the first H-OH overtone absorption band (Figure 3). This high SD was caused by wide variation in the spectral fingerprint due to water.

Figure 3. Standard deviations of absorbance values.

Calibration

The performances for moisture content calibration equations (Table 1) developed on each instrument were very close and highly satisfactory. Both instruments gave a RPD higher than 7, which means that predictive models can be used as routine analyses for an accurate moisture content determination.

Table 1. Performance statistics for coffee bean moisture content calibration equations.

<table>
<thead>
<tr>
<th>Spectrometer</th>
<th>SEL (%)</th>
<th>SEC (%)</th>
<th>R²</th>
<th>SECV (%)</th>
<th>RPD = SD/ SECV</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-Two</td>
<td>0.05</td>
<td>0.16</td>
<td>0.98</td>
<td>0.17</td>
<td>7.14</td>
</tr>
<tr>
<td>Foss 6500</td>
<td>0.05</td>
<td>0.12</td>
<td>0.99</td>
<td>0.17</td>
<td>7.28</td>
</tr>
</tbody>
</table>

The similar performances in terms of fitting were confirmed when predicting from the validation set of samples (Table 2 and Figure 4). For the 35 samples, the RPDs expressed as
the ratio of SD to SEP were higher than 6; 6,5 for the X-Two and 6,7 for the Foss. The SEP values were close to SECV (0,19% and 0,18% for SECV equal to 0,17%), which means that the models are robust.

Table 2. Performance statistics for prediction of coffee bean moisture content using two different calibration equations.

<table>
<thead>
<tr>
<th>Instrument</th>
<th>SEP</th>
<th>R²</th>
<th>Bias</th>
<th>SEPc</th>
<th>slope</th>
<th>RPD</th>
</tr>
</thead>
<tbody>
<tr>
<td>X-Two</td>
<td>0,19</td>
<td>0,98</td>
<td>0,06</td>
<td>0,18</td>
<td>0,94</td>
<td>6,47</td>
</tr>
<tr>
<td>Foss 6500</td>
<td>0,18</td>
<td>0,98</td>
<td>-0,03</td>
<td>0,18</td>
<td>0,98</td>
<td>6,68</td>
</tr>
</tbody>
</table>

The difference between the instruments in terms of accuracy and robustness was due to the spectral range of the instruments: the wider range of the FOSS gave more information about samples (after 1700 nm) which allowed a better separation between noise and relevant information. This was illustrated by plotting the PLS loadings (Figure 5), which showed a supplementary band at 1940 nm with high coefficients for the FOSS instrument.

![Figure 4. Scatter plot of moisture reference and NIR predicted values.](image)

**Figure 4. Scatter plot of moisture reference and NIR predicted values.**

![Figure 5. Loadings for the first PLS factor from the X-Two and FOSS equations.](image)

**Figure 5. Loadings for the first PLS factor from the X-Two and FOSS equations.**

**CONCLUSION**

The moisture content calibration obtained with the X-Two spectrometer could be used on-line at the end of the roasting process to control coffee bean moisture content with high accuracy. The implementation of such an instrument on-line will allow monitoring of water injection at the end of the roasting process and furthermore improve quality control over time. This approach could be expanded to include colour prediction, which would allow control of roasting degree.