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IN-HOUSE EXPERIMENT

ANALYZING PEACH RIPENESS: LINKING SUGAR CONTENT TO ABSORBANCE SPECTRA

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BACKGROUND INFORMATION

Peaches belong to a family of fruits known as stone fruits. Characterized by the large single seed in their center (also known as the stone or pit), stone fruits also include apricots, cherries, raspberries, olives, and even coconuts. Since most stone fruits will not ripen after being picked, it is essential that they are harvested at peak ripeness, which also means these fruits have a small window for consumption. Determining ripeness when buying stone fruits in a store can be done informally by giving the fruit a small squeeze (a hard fruit indicates that it is not fully ripe) or by smelling the fruit (the more aromatic the fruit, the riper it is).

While this is feasible for a customer buying a few pieces of fruit, how can distributors sort fruits to only include the highest quality, ripest fruits in their shipments? Since ripeness itself is somewhat subjective and difficult to quantify, it is often correlated with the sugar content in a fruit, which increases as the fruit becomes riper. Sugar content can be defined by the unit Brix (where 1 Brix is 1 g of sucrose in 100 g of solution) which can be easily measured with a device called a refractometer. Unfortunately, this sugar content measurement requires juice from the individual fruit, which is considered destructive in that the fruit is no longer in a condition to be sold to consumers. For commercial operations who are interested in characterizing and sorting fruits of various types by the ton, non-contact near infrared spectroscopy can be used to measure brix accurately and efficiently. Around the world a variety of companies produce near infrared fruit sorting systems which are capable of characterizing hundreds of units of fruit per minute. Avantes is a major supplier to this industrial application with systems deployed around the world. Instruments of choice for this application are our AvaSpec-HS2048XL-EVO and the AvaSpec-ULS2048XL-EVO which both have exceptional sensitivity in the wavelength range of interest from 600-1100 nm along with high speed sampling and data transfer capabilities.

This simplified experiment aims to demonstrate this non-contact technique for predicting the sugar content, and therefore the ripeness, within peach samples using this same spectroscopic technique. Peach samples were illuminated in free space with an overhead tungsten halogen lamp and were measured multiple times on a turntable using a bare 600 micron core fiber optic cable (FC-UVIR600-1-BX) connected to a spectrometer (AvaSpec-ULS2048XL-EVO). The sugar content of the peach samples was separately determined using a refractometer. The spectroscopic measurements were paired to the refractometer sugar measurements to create an algorithm to correlate the differences in the spectra to a level of sugar content. We then tested additional samples to determine the accuracy of our generated algorithm.

FIGURE 1 Peach samples used for this experiment. The eight peaches in the back row were those used to create the correlation between the measured spectra and sugar content, and the four peaches in the front row were those tested to determine the accuracy of our algorithm.

DESCRIPTION OF SPECTROSCOPY SETUP

The setup for this experiment (Figure 2) was based around the AvaSpec-ULS2048XL-EVO. This device combines exceptional quantum efficiency with high-speed communication. Unlike many back-thinned CCD spectrometers with two-dimensional arrays, the ULS2048XL-EVO has large monolithic pixels of 14x500 microns with exceptional efficiency in the UV range (200-400 nm) and NIR range (950-1160 nm). This instrument features an electronic shutter that enables integration times as low as 2 microseconds and has a detector collection lens available that can further enhance sensitivity up to 60% when combined with larger core fibers. This device features our AS-7010 electronics board which offers fast USB3.0 and gigabit ethernet communication, has an exceptional signal-to-noise ratio of 525:1, and can be customized with a wide range of slit sizes, gratings, and fiber optic entrance connectors for a variety of application needs. The instrument used in this experiment had a wavelength range of 600-1100 nm and a 200-micron slit installed.

The light source used for this experiment was a commercially available incandescent (tungsten halogen) 60-watt lamp. With a brightness of 1070 lumens, this light source setup resembles what may be used in a large-scale fruit processing operation.

Other accessories used for this experiment included a 600-micron core fiber optic cable to directly measure the peach samples, a WS-2 white reference tile that was used as a reference material, a turntable to rotate each peach sample for randomization and sampling at multiple measurement points, and a clamp and clamp stand to hold the fiber and overhead lamp in place.

FIGURE 2 Experimental setup. One end of the fiber optic cable is connected to the spectrometer while the other is clamped and pointed at the peach sample. The peach samples are illuminated by the overhead lamp and are rotated via the turntable to take multiple measurements per sample.

DESCRIPTION OF METHODOLOGY

12 peach samples were used in total, with eight being used to create the algorithm correlating absorbance spectrum to brix measurement and four used to verify the accuracy of the algorithm. The peaches were stored in a refrigerator to prolong the timeframe for their ripeness but were left in a room-temperature environment for a minimum of four hours before measurements were taken to ensure the sample temperature had minimal effect of the recorded data. Each sample was individually placed on the turntable center and allowed to spin freely under the overhead lamp. 10 measurements of each peach sample were taken to quantify the average spectrum of each sample, create more data points for the algorithm creation, and determine if any measured spectra were outliers that could skew the algorithm. Each peach sample was then sliced in two opposite positions on the fruit, and the fruit of each slice was individually squeezed onto the refractometer window to determine the Brix value of each slice. The two Brix values for each peach sample were averaged. Because the spectra used were absorbance spectra, a reference measurement was taken using our WS-2 white reference tile at a similar distance and angle as the peach samples.

For data analysis, we used the absorbance mode in Panorama, a third-party software from LabCognition of Germany that is compatible with our spectrometers and has custom plugins designed specifically for our instruments. Absorbance measurements require both a dark measurement and a reference measurement to compare the sample measurements against. The dark measurement was taken with the overhead light off and no peach on the turntable, but with ambient light still present so it could be subtracted from the sample measurements. As stated previously, the reference measurement was taken with the overhead lamp on and our WS-2 white reference tile at a similar measurement distance and angle as the peach samples. The integration time was set to 2 milliseconds, which can be adjusted to increase or decrease the amount of light being measured at one time and affects the overall magnitude of the reported spectrum. Averaging was set to 1, meaning each spectrum corresponds to one unique measurement. Within the Panorama software, a calibration was created using the included PLS1 model, with the measured brix values as the valuation property. After selecting default values for the spectral range for the calibration and the number of factors for analysis and calibration, the initial algorithm was generated. The data included was adjusted to remove any outlier spectra to give the most accurately predictive algorithm based on the measurements of the first eight peach samples. Lastly, the additional four peach samples were measured, with the algorithm's predicted sugar content values compared to the values measured with a refractometer.

TEST DATA AND RESULTS

Displayed below are the spectra of the eight peach samples used to create the algorithm, showing the range of spectral data:

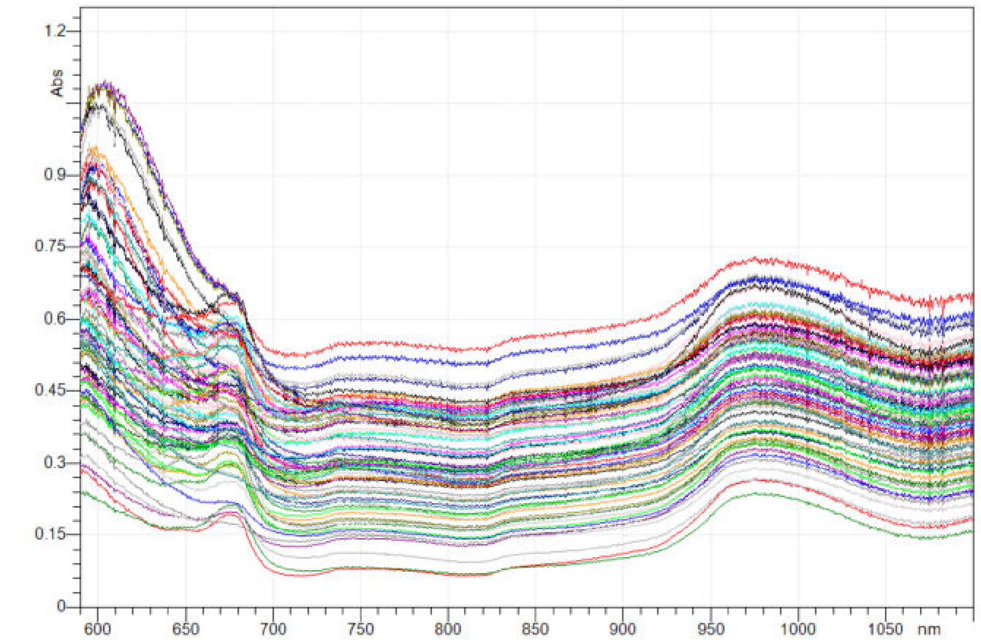

FIGURE 3: Absorbance spectra of eight peach samples used to create algorithm correlating spectra to sugar content

Utilizing all 80 measurements, the generated algorithm predicted the sugar content of every included sample measurement. In the table below, 10 of these predicted values are given and compared to the actual measured sugar content values for the sample measurement.

Sample Measurement	Actual Brix Value	Predicted Brix Value	Absolute Difference
Peach1_01	9.5	11.235	1.735
Peach2_01	10.9	11.224	0.324
Peach3_06	10.5	11.264	0.764
Peach3_09	10.5	11.287	0.787
Peach4_01	9.7	11.326	1.626
Peach4_03	9.7	11.177	1.477
Peach5_09	11.0	11.093	0.093
Peach6_03	11.7	11.316	0.384
Peach7_06	12.0	11.205	0.795
Peach8_05	13.3	11.261	2.039

It is clear by this table that the initial algorithm included too many outliers that a correlation between spectra and sugar content could not be generated. Indeed, below is the plot of the predicted-versus-actual Brix values along with the linear fit to the data and the R2 value of the linear fit:

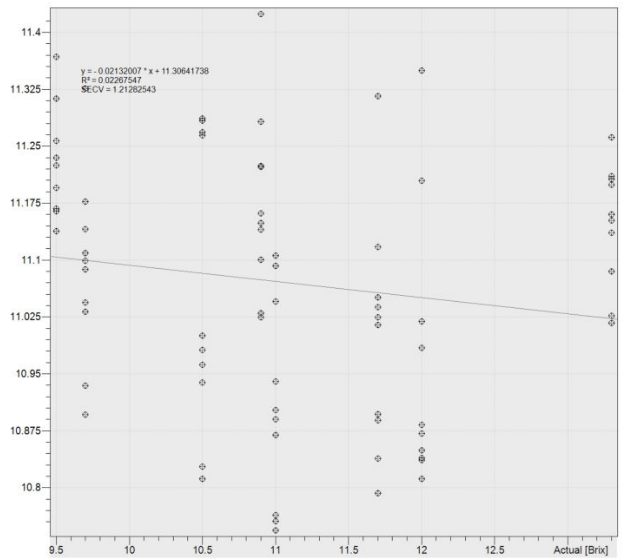

FIGURE 4: Plot of the predicted-versus-actual Brix values with thelinear fit to the data and R⁻² value of fit

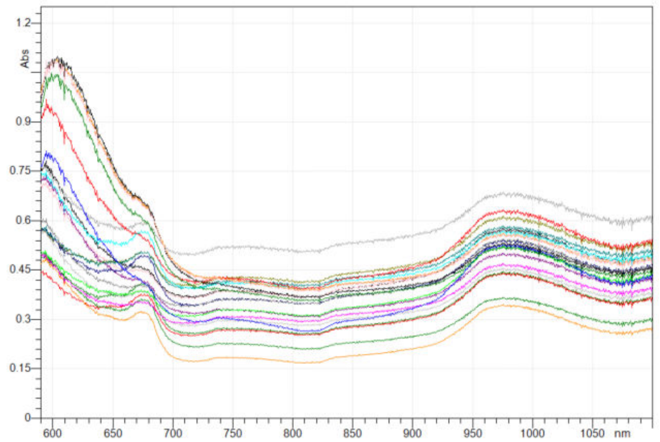

FIGURE 5: Absorbance spectra of eight peach samples used to create updated algorithm correlating spectra to sugar content, with outlier spectra removed

Based on the almost-zero R^2 value, it was determined that a significant number of spectra were outliers and had to be removed. After removing outlier spectra, a total of 23 spectra were used to generate an updated algorithm. The spectra of the non-outlier measurements are shown in Figure 5.This updated algorithm produced the following results for predicted sugar content compared to actual sugar content in 10 sample measurements

Sample Measurement	Actual Brix Value	Predicted Brix Value	Absolute Difference
Peach1_05	9.5	9.630	0.130
Peach1_07	9.5	9.627	0.127
Peach2_02	10.9	10.815	0.085
Peach3_01	10.5	10.629	0.129
Peach3_08	10.5	10.396	0.104
Peach4_07	9.7	9.791	0.091
Peach5_06	11.0	10.882	0.118
Peach5_07	11.0	11.106	0.106
Peach6_08	11.7	11.669	0.031
Peach7_02	12	12.048	0.048

Lastly, this updated algorithm provided a much closer linear fit to the data set, shown in the plot below along with the R2 value of the linear fit:

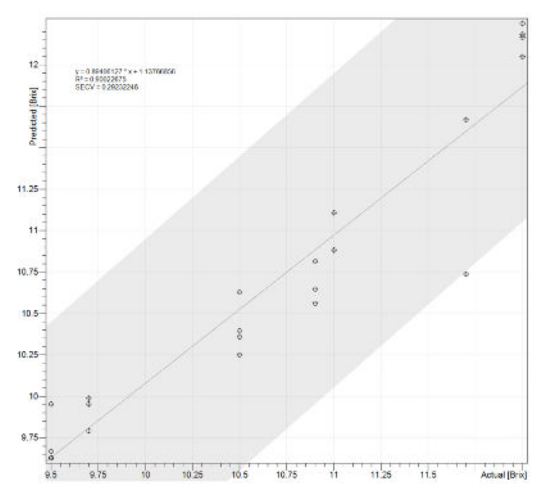

FIGURE 6: Plot of the predicted-versus-actual Brix values with the linear fit to the data and R⁻² value of fit

ANALYSIS AND CONCLUSION

As stated previously, including all the measured spectra in the algorithm calculation resulted in no correlation between absorbance spectra and Brix measurement. This is because too many outlier spectra were included in the calculation. After removal of what were considered outlier spectra, the algorithm very closely predicted the sugar content of each peach sample. Unfortunately, all measurements for sample peach eight were considered outliers based on the spectra and measured Brix value, so this fruit sample was excluded. With the algorithm closely predicting the sugar content of the peach samples used to create it, additional measurements were taken of the four other peach samples to verify the accuracy of the algorithm. The same method was used, with ten absorbance measurements taken of each peach sample followed by two slices cut from each peach on opposite sides of the fruit to determine actual sugar content with the refractometer. 10 of the results are given in the table below:

Sample Measurement	Actual Brix Value	Predicted Brix Value	Absolute Difference
Peach9_03	12.5	12.252	0.248
Peach9_08	12.5	12.262	0.338
Peach9_09	12.5	12.264	0.336
Peach10_01	9.6	10.135	0.535
Peach10_02	9.6	9.618	0.018
Peach10_08	9.6	9.819	0.219
Peach11_01	12.8	10.964	1.036
Peach11_08	12.8	10.900	1.900
Peach12_05	11.6	10.037	1.563
Peach12_06	11.6	10.035	1.565

The results show a high degree of accuracy in predicting the sugar content of peach samples 9 and 10 but are much less accurate for samples 11 and 12. This could be due to the fact that samples 11 and 12 were beginning to show signs of rotting, including slightly wrinkled skin, whereas the inner juice from the fruit slice may still contain the same level of sugar. Alternatively, this may be an indication that creating such a predictive model requires a larger sample size and additional pieces of equipment to take even more scans of the fruit.

CONCLUSION

In conclusion, the present experiment highlights how absorbance measurements can be utilized to predict the sugar content, and therefore ripeness, of peach samples. It should be noted that even the four samples used to determine the accuracy of our algorithm did include outlier spectrum that were excluded, and more sophisticated methods would need to be implemented to decide which spectra are considered valid or outliers. Since fruit sorting is most often an in-line process with fruit moving quickly, multiple fiber optics and spectrometers are utilized to collect high amounts of data and determine a true average spectrum for each fruit. While this simple experiment demonstrated the capability of this technique, significant data acquisition and modeling is required to develop robust and accurate models which can be used in a commercial environment for high speed fruit sorting. The AvaSpec-HS2048XL-EVO and AvaSpec-2048XL-EVO are ideal candidate instruments this application which requires NIR sensitivity and high speed acquisition capabilities. Please contact and Avantes sales Engineer for more information on this application and Avantes instruments for fruit measurements.

CONTACT

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