

Application Note: G01

Does Sample Temperature Affect NIR Accuracy with the Unity Scientific SpectraStar NIR Flour Analyzer?

Introduction

Near Infrared Spectroscopy (NIR) is a widely accepted tool for quality control in the flour milling industry. Typical NIR analysis is conducted on wheat flour during the milling process to manage flour quality for moisture, protein, and ash concentrations. Process specifications on moisture, protein, and ash are rigid to maximize product yield. Therefore, NIR accuracy is a crucial element for the flour miller to evaluate product quality and maintain process controls.

The purpose of this study is to evaluate the effect of flour temperature variation on NIR accuracy in a typical flour milling environment. If a miller collects a flour sample directly off the mill, the sample is hot to the touch. The question arises; will the miller obtain an accurate NIR analysis on this hot flour sample if the NIR has been biased to samples analyzed at room temperature? Additionally, will the miller obtain the same NIR result if the same sample is allowed to cool to room temperature? These questions are important to the flour miller because they do not consistently analyze flour samples on the NIR at the same temperature.

Experimental Design

This experiment was conducted in cooperation with a major flour milling company in the United States. The following steps were performed on 11 independent flour samples during one week of production:

1. Sample was collected “in-process” and placed in a sealed metal container.
2. Sample was immediately analyzed on the Unity SpectraStar 2200.
3. Sample was subsequently analyzed at time intervals of 1, 2, 5 10, 20, and 30 minutes.

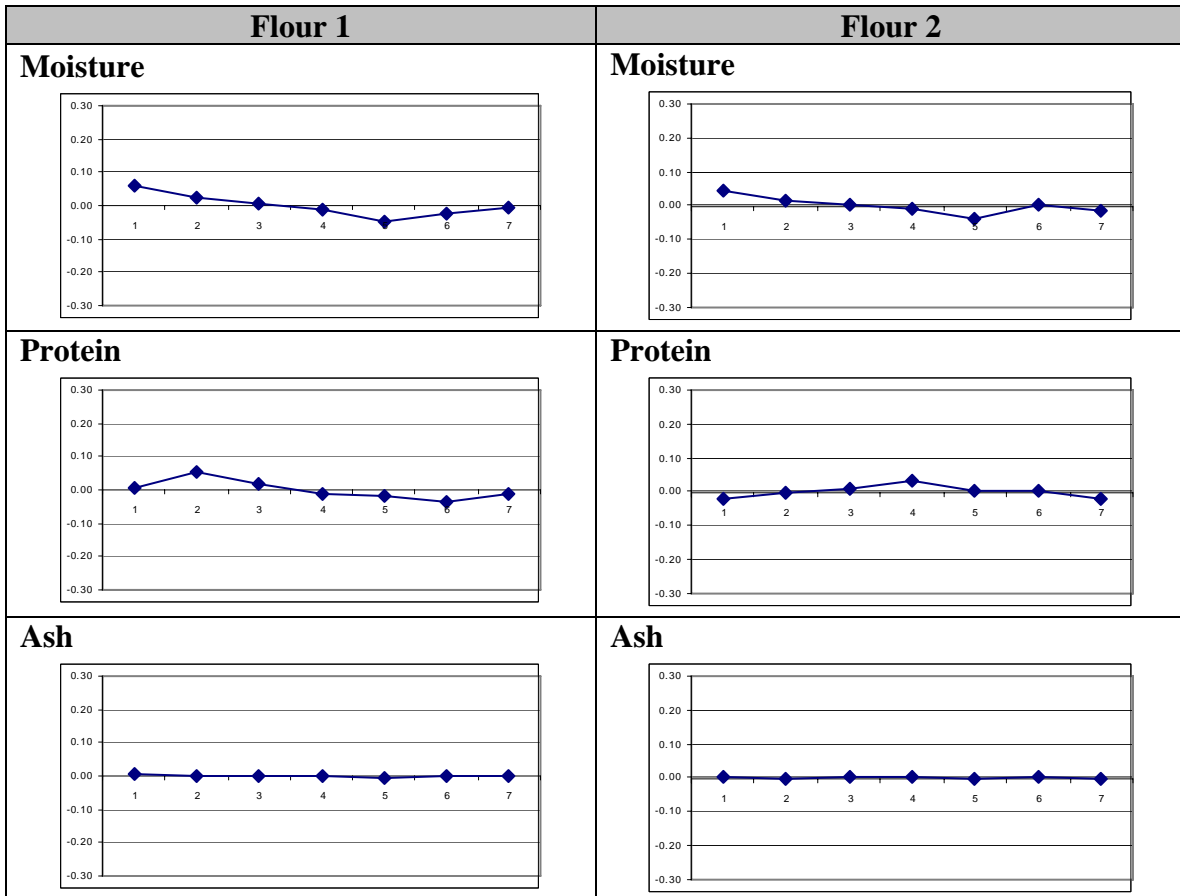
The intention of this experimental design is to simulate a flour miller’s experience if the flour sample is immediately analyzed on the NIR at a higher temperature versus if the sample is analyzed within a 30 minute time frame as the sample cools to room temperature.

Data Analysis

The resulting spectra were compared against two sets of flour calibrations for moisture, protein, and ash. The first calibration set is called “Flour 1”, the second calibration set is called “Flour 2”. Flour 1 is a set of flour calibrations generated from flour samples at room temperature. Flour 2 is a set of flour calibrations generated from all the samples in Flour 1 plus the temperature variation data gathered from this study. The predictions for each sample as calculated from calibration sets Flour 1 and Flour 2 were plotted to evaluate prediction trending as the samples cooled to room temperature. Then the standard deviation was calculated for each parameter of every sample to determine if the Flour 2 calibration set significantly outperforms the Flour 1 calibration set.

Results

The following six plots represent prediction trending as one sample was allowed to cool to room temperature. This sample represents the general trend for all samples. As can be seen from these plots, there is not a significant change in prediction as the sample cooled, nor is there a significant change between calibration sets Flour 1 versus Flour 2.



The following table illustrates the standard deviations for each sample as analyzed during the seven time intervals and predicted against Flour 1 and Flour 2. Overall, the standard deviations for calibration set Flour 1 and Flour 2 show good accuracy. There is no improvement using Flour 2 moisture. There are small statistical improvements using Flour 2 for protein and ash.

Sample	Flour 1 Moisture	Flour 2 Mositure	Flour 1 Protein	Flour 2 Protein	Flour 1 Ash	Flour 2 Ash
1	0.075	0.090	0.096	0.131	0.0175	0.0044
2	0.049	0.038	0.087	0.048	0.0116	0.0118
3	0.042	0.033	0.133	0.073	0.0114	0.0064
4	0.034	0.026	0.030	0.019	0.0036	0.0028
5	0.044	0.070	0.124	0.080	0.0178	0.0053
6	0.028	0.034	0.148	0.038	0.0020	0.0093
7	0.049	0.033	0.059	0.036	0.0054	0.0032
8	0.046	0.057	0.049	0.046	0.0036	0.0055
9	0.042	0.055	0.031	0.157	0.0046	0.0030
10	0.034	0.074	0.122	0.076	0.0192	0.0072
11	0.038	0.024	0.060	0.055	0.0031	0.0025
Average Standard Deviation	0.044	0.049	0.083	0.069	0.0091	0.0056

Conclusion

The data in this study shows the Unity Scientific SpectraStar flour calibrations are capable of accurately analyzing moisture, protein, and ash for samples directly off the mill and while the samples cool to room temperature. The flour samples do not appear to dramatically trend in prediction values as the flour cools. Additionally, including the temperature variation samples into the calibration model has only a small effect on prediction results for samples of varying temperatures.

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