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Mark/E. Stark

TRIP REPORT
NORRIS & WILLIAMS (10/12/77)

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DISTRIBUTION

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Purpose: To obtain the latest information about Norris' new data treatment and its effect on his presentations at A²C² meeting.

Norris claims to have "stumbled across a magic data treatment" that is the combination of absorbances as follows:

$$\frac{(R_{2180} \text{ nm} - R_{2120} \pm 2 \text{ nm}) / (R_{2180} \text{ nm} + R_{2120})}{(R_{2280} \pm 7.5 \text{ nm} - R_{2230} \text{ nm}) / (R_{2280} + R_{2230})}$$

or the equivalent expression:

$$\frac{\log \frac{1}{R_{2180}} - \log \frac{1}{R_{2120}}}{\log \frac{1}{R_{2280}} - \log \frac{1}{R_{2230}}}$$

Since $(R_{2180} + R_{2120})$ is almost equal to $(R_{2280} + R_{2230})$ for a large range of samples, Norris has also used $(R_{2180} - R_{2120})$

$$(R_{2280} - R_{2230})$$

with almost as good results.

Of all the data treatments he has tried, this treatment is the best on the basis that for protein in wheat when calibrating with one data set and using the calibration to predict the protein in a different set, the results obtained are the most insensitive to moisture variation. He can consistently predict protein in wheat with a standard error of prediction (SEP) less than 0.4% (average 0.35%), regardless of the moisture range in his calibration samples. The average SEP for all particle size files (different types of grinders) is 0.45 as compared to 0.33 for D^2OD/D^2OD_{ref} .

Norris has simulated both InfraAlyzer and Neotec units and has made tables of the standard errors obtained on prediction when calibrating on one data set and using that calibration to predict the other data sets. Figure 1 contains the table of these standard errors on prediction for Norris' simulated InfraAlyzer and Neotec units. Figure 2 is the summary tables that he plans to present at A²C², comparing InfraAlyzer and Neotec units to each other and to those data treatments that didn't bomb completely. He intends to show "both how good and how bad" both company's instruments are.

Both Norris and Williams feel that this new data treatment should be incorporated into instruments. Phil Williams is interested in having InfraAlyzer units in Canada modified for the new data treatment and is willing to pay for modification for some of his units and share the data obtained from these units with us on the basis of a joint experiment.

There was some discussion of instrument drift and its causes. According to Phil Williams, Neotec 41 units have been known to drift as much as .8%. He implied this is sample drift. Norris had found some information in the literature concerning band shifts with temperature; and for moisture, the absorptivity at a given wavelength can change by as much as 0.1%/°C. While this undoubtedly contributes some error to the system, Norris feels that this has only a minor effect, as moisture in corn has been predicted with a standard error of .07%.

Norris did not consider temperature variations in his studies of the new data treatment.

Miscellaneous

The extraneous datum found in Norris' data sets is a soft wheat sample.

Phil Williams recommends using a 35 mm film canister as a scoop for taking grain for grinding, as it holds $25 \pm .3$ g of wheat.

Norris currently has two people temporarily working in his laboratory with the Fourier Transform spectrometer, one is from Neotec using the FT system to test a monochromator. The other is from Lambda instruments Corp. in Lincoln, Nebraska; he is staying for 4 months to learn about FT spectroscopy, reflectance spectroscopy and their application to grain measurements.

Phil Williams' sealed cell needs grease on the threads to maintain the seal, the gasket is unnecessary.

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