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Purpose of trip: To use Norris' computational facilities to reanalyze his moisture data and to obtain a copy of this data for further analysis in-house.

After some discussion concerning how to best modify his programs, we rewrote the subroutine for applying a filter function to spectral data and inserted it into Norris' program. They made several useful suggestions on how to speed up the subroutine that we can incorporate into our own spectral search programs.

We then took Norris' moisture data files for 4-12% moisture and created the new files containing spectral data modified by a filter factor listed in Table 1. The filter shape chosen was IRI's design "C". We also created a file that contained the combined data from the two files, 1W250A and 1W450A, "high" and "low" moisture files.

New Math

The program we used permitted us to specify 3 of the wavelengths for the "new math" calculation and it would optimize the fourth. I initially specified 2100, 2180 and 1680 nm, but the best fit obtainable had a SEE of greater than .35% protein when calibrating on all 6 files, initial computer runs were made to determine the optimum wavelength spacing and center wavelengths for the filter-modified data. The optimums were found to be 21472A (numerator) and 22656A (denominator) ±20 points (32 nm), i.e.: 21792 and 21152 nm (numerator) and 22976 and 22336 nm (denominator) The results of predicting each sample set using these wavelengths is shown in Table A.

I then investigated the effect of forcing the use of standard InfraAlyzer wavelengths. When the wavelengths specified were 2180, 2120 and 1680 nm or 2180, 2117 and 1680 nm, the computer found 2304 nm to be the optimum wavelength.

The results of using these two sets of wavelengths are shown in Tables 2 and 3. Calibrations were done on files 1W250F, 1W350F and 2W450F as representative "high", "medium" and "low" moisture data sets; and also on a data set comprised of all six files combined. For each calibration, each data set was predicted individually, with the SEP’s listed.

InfraAlyzer Simulations

Calibrations were done on data set 1Wl00F only, as calibrations on a single set, with only a small moisture range resulted in very large biases when predicting the other sets, several sets of wavelengths were tried and the results of predicting the four sets not in the calibration set are listed in Table 4A. More than four wavelengths could not be used at a time because the computer would automatically drop one of the wavelengths as "non-significant". An example of this is also included in Table 4. When each absorbance was divided by the absorbance at 2275 nm, the computer deleted A1940/A2275 from its prediction set.

I was also not able to do a computerized search for a fourth optimal wavelength. However, I was able to search by selecting 4 wavelengths at a time and looking for the optimum SEE. On this basis, the best fourth wavelength was 1670 nm, with a SEE of .199. The results of predicting the other sets with the wavelength combination 1670, 1680, 2117, 2180 nm is shown in Table 4B.

Misce1laneous

1. Norris noted that the sets 2W250 and 2W350 always gave worse results than the other data sets. This probably means that they are in fact running on a different calibration than the other sets.

2. Neotec brought a 31 and 41 into Norris' laboratory and hooked them to Norris' computers to do an optimization on the pulse points. The 31 did not perform satisfactorily. Norris didn't remember the exact figure, but said the SEP from the 31 with new math was .4 or .5. The 41 performed satisfactorily between the 8-12% moisture ranges. I told Norris I thought we could probably predict within FGIS spec in that moisture range with our universal calibration.

3. Norris had one of the new DJ units in his lab. The covers were all locked down. The drawer had a tendency to bounce when being closed; the detent on opening was more pronounced. There was a fan and air filter on the left hand side. Removing the filter might have made it possible to see inside through the fan but it was too dark inside to see anything without a flashlight. Computer "hung up" when drawer was closed without a sample.

4. Norris said the 8-filter decision of FGIS was probably brought on by us and DJ asking about it. Norris feels that FGIS should take the "black box" approach and specify only performance and not care "if you can make the measurement with only one filter".

5. Norris did not temper samples up except initially. After a "very long" of whole grain tempering to 14-15%, wheat was ground on the Wiley Mill to 14% moisture, on the Udy to 12% moisture, air dried to 9-10% moisture, vacuum dried to ~4% moisture and oven dried to ~.5% moisture.

6. I managed to bring up the point that the moisture correction via new math degraded the otherwise much better results obtainable. During the ensuing discussion, Norris seemed shocked when I pointed out that there was absolutely no hard evidence that the occasional outliers observed in the field were, in fact, due to moisture variations.

7. Norris does not plan to do any further InfraAlyzer simulations, although he has said previously that he does plan further investigations of other data treatments.

8. When I arrived, a salesman from Princeton Applied Research was obtaining high and low oil soybean samples from Norris to see if he could tell the difference on their optoacoustic spectrometer. Norris thinks as good results could be obtained by using a technique involving the same irradiation as used in optoacoustic spectroscopy, but detect the temperature changes of the sample by measuring the emitted IR radiation with PbS instead of the sound radiated.

9. There was some discussion of why the instruments don't reliably work satisfactorily on new math when all the simulations say they should. Norris feels it might be due to sample differences although he has used four different sample sets without problems. He does not feel that the simulations are faulty even though I pointed out the differences in noise, linearity and drift characteristics between his spectrometer and field instruments.

10. We have all Norris moisture data (more than the six sets I used on his computer) on HP9825 cassettes.

11. Norris plans to investigate the new DJ unit as a whole wheat machine. He feels there is a market for a whole wheat machine with a standard error of .5%.

Conclusions and Recommendations

1. The results obtained give us a basis for claiming to FGIS that, if new math works at all, then current InfraAlyzer wavelengths should perform satisfactorily, except for replacing 2100 nm with 2117.

2. We proceed with all dispatch to transfer Norris' data to our computer.

3. We send Norris HP cassettes to replace the one he gave us with his data.

4. We keep a close eye on his future data treatment experimentation.

HM/po
Attachments

Table A

(Optimum set) λ = 21792, 21152, 22976, 22336

Calib. File	Predicted File 1W250A	1W350A	1W450A	2W250A	2W350A	2W450A
All six	.236	.252	.236	.285	.316	.235

Table 1

1W250F	12.5%
1W350F	9%
1W450F	4%
2W250F	12.5%
2W350F	9.5%
2W450F	6%
1W100F	1W250 + 1W450

NEW MATH

Table 2

λ = 21216, 21800, 22304, 22810

Calib. File	Predicted file					
	1W250	1W350	1W450	2W250	2W350	2W450
1W250	.206	.262	.265	.3239	.334	.275
1W350	.232	.235	.224	.310	.353	.246
1W450	.225	.235	.225	.310	.348	.245
All 6:	.209	.240	.226	.320	.332	.244
SEE =	.262					

Table 3

λ = 21170, 21800, 22304, 23100

Calib. File	Predicted file					
	1W250	1W350	1W450	2W250	2W350	2W450
1W250		.24	.308	.334	.327	.255
1W350	.209		.343	.316	.331	.276
1W450	.232	.276	.357	.381	.330	
All 6:	.206	.246	.296	.342		.50
SEE =	.266					

Table 4A

InfraAlyzer Simulations

A Combos	1W350F	2W250F	2W350F	2W450F
	Data Set Predicted			
2100, 2180, 1680, 1940	.498	.522	.436	.298
2117, 2180, 1940, 1680	.266	.488	.474	.288
2100, 2180, 1680	.596	1.06	1.17	.402
2100, 2180, 1680, 2275	.515	.543	.470	.324
2100, 2180, "1940", 1680 each ÷ 2275	.496	.500	.429	.312

Table 4B

1670, 1680, 2117, 2180 (SEE = .199)	.248	.506	.495	.334