

TECHNICON INTERNAL MEMO

To: J. Psotka  
From: H. Mark  
Date: Aug. 20, 1984  
Subject: Trip report, Diffuse Reflectance  
Symposium at Wilson College,  
Chambersburg, Pa.

Copy: D. Burns  
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J. Judge

The meeting was an outstanding success in all respects. The representatives of all the -instrument companies behaved like gentlemen and scientists, except for Janet Casciero who behaved like a lady. The debates over the scientific content of the talks never once degenerated into a shouting match between the companies.

Despite a couple of minor SNAFUs the hospitality suite was a resounding success. I have to admit that before we went there I had some reservations concerning the wisdom of separating ourselves from the main group, however, I have to compliment Howard on what was nothing less than a stroke of genius. With Dennis as the genial host, and the rest of us present to answer technical questions, we came off as good, hardworking scientists, like the rest of them. Even more important, our providing a place where everyone could assemble to discuss conference (and other) business when no formal session was in progress was recognized and appreciated by all conferees, one of whom stated "more business was conducted after 10:30 than during all the sessions". When I rose Thursday evening on behalf of Technicon to accept their thanks, I felt very proud to be a part of such a class operation. We really came off like heroes. The only way we could top this next time would be to host a suite such as this in conjunction with the other companies. Not only would this save money, but it would avoid the potential disaster of having one of the other companies also set up a suite, thus dividing the conference. Besides, there was plenty of glory to go around; there is a place for competition and a place for cooperation (more of this later).

Some of the following comments are general, some are directed toward the appropriate individual for action:

Jim P. and Howard V.: Harald Martens would like to see the comments that Dr. Hoerl made concerning ridge regression and my response. May I send this to him. Please respond ASAP, (also see comment below regarding Harald's new statistic)

Rick Benson (Cargill) is working on a discriminant analysis program for his own use. I demo'ed our package for John Rose and Bill Hrushka; I invited Rick also, but he didn't show. John appeared possibly interested in purchase (I think).

Tom Long (R. J. Reynolds) is having trouble transferring data off an HP-85 Plus tape. I will send him a copy of the file structure and offer him telephone assistance.

Harald Martens' talk dealt with data pretreatments, among other topics. He

showed an improvement of a factor of two in accuracy by choice of the proper pretreatment. However, it was clear that the proper pretreatment is not always obvious, and certainly not always the same from sample type to sample type. Harald felt that many of the various data analysis methods can give equivalent results (multiple regression, principal component analysis, fitting spectra, Fourier transforms, partial least squares), but some have other advantages (e.g. Principal components and partial least squares can reduce multicollinearity), and there was general agreement on these points.

As Don B. noted in his trip report, there was an upsurge of interest in certain specific software packages. Fourier Transform and Data transfer shared top billing on the list; Partial Least Squares came in second. Peter Griffiths told me he knows of a Fourier Transform program in FORTRAN that only takes a dozen or so lines; I will ask him for the reference on this. Everyone seemed interested in a means of transferring data among all NIR users. I think Karl could be persuaded to act as a clearinghouse for data, but he would need equipment.

Jim P. and Apps group: I have been remiss in watching out for ways to improve calibrations. Tom Nolan presented an interesting division of data analysis techniques into what he called "enumerative<sup>M</sup>" and "analytical". He then pointed out that the methods that have been proposed in the past for analysis are all enumerative, however sophisticated they are. He presented data for one of what he called analytical techniques, the particular case being one in which plotting residuals as a function of the order in which the reference laboratory analyzed the samples revealed a week-to-week shift in the lab values; essentially he created a control chart for the residuals. We have known about doing this kind of stuff for a long time; we need to apply such techniques more often. Other such techniques we know about are the use of indicator variables and plotting the cumulative normal distribution curve for data to reveal problems.

Karl Norris divided the various techniques somewhat differently: he called the two categories "population sampling" and "absorption band spectroscopy". Basically, population sampling relies more heavily on statistical approaches; the other relies more on spectroscopic considerations.

A number of books and other major works on NIRA are available or soon to become so:

"Food Research and Data Analysis" by Harald Martens and Helmut Russwurm, Elsevier Science Publishing Co., Inc. (1983)

"Near-Infrared Reflectance Spectroscopy - Principles and Applications" edited by Phil Williams - to be published soon

A review of NIHA soon to be published in Applied Spectroscopy Reviews was announced. Ed Stark arranged to receive a pre-publication copy. Ed, don't forget to distribute this to everyone when you get it.

Harald vaguely mentioned a method that might be better than discriminant analysis, that would be based on principal components; I discussed this with him and he became less sure of his ground; apparently it was an idea he hadn't worked through yet and didn't really know if it would pan out.

Jim P. and Howard V.: Woody Barton has been having a problem transferring data out of his I/A 500 in Lelystadt, Netherlands. While he did not know the ROM version he has, it sounded like he ran into the communications bug we found in the early versions of the I/A 500 firmware. Since Woody is a

key member of the forage network, it behooves us to get him fixed up ASAP.

John J.: Dave Funk gave a good summary of considerations pertaining to human engineering of an instrument. He discussed many items that are useful; one very simple one he brought up is the use of a beeper to signal the END of an analysis to combat operator inattention. Another item that generated interest at the meeting was the concept of a "bare bones" instrument that requires an external computer; this makes future upgrades simple and cheap. See me for a fuller list of his discussion.

Don Webster divided the NIR spectrum into three regions, the part we cover corresponds to what he called regions I and II (the break is about 1900 nm). Region III covers 850 to 1100 nm; they do a lot of work with slurries (e.g., meat, etc.) in region III.

#### Future conferences\*

Karoly Kaffka announced an international NIRA conference to be held in Budapest, Hungary on May 12-16, 1986

Franc Greem (or Grum, I have two different spellings) of the Rochester Institute of Technology offered to organize the next Diffuse Reflectance Symposium at R.I.T. Apparently he just got a large infusion of money to set up a reflectance laboratory (see below) and wants to make the scientific community aware of it.

Fred McClure offered to organize the next Diffuse Reflectance Symposium at Raleigh. This met better acceptance than Franc's offer, but the general feeling was: Raleigh, in the SUMMER?

Woody Barton was nominated by Dave Wetzel as the next organizer, and probably will get stuck with it. Questionnaires will be sent around in the near future, as was done last time.

Peter Griffiths reminded the group about the conference on computerized infrared spectroscopy in Ottawa next year.

Bob Rosenthal (Trebor) had his instruments on display and gave a presentation relating to them. Basically he uses silicon detectors and 12 IR-emitting diodes; mainly his instruments measure moisture. He has larger temperature sensitivity at the shorter wavelengths than we do; he combats this by placing a thermistor in the sample cup and including temperature in the calibration.

Peter Griffiths described his work in mid-IR reflectance - great care in sample preparation is needed for reproducible readings. During lunch following Ed's talk he mentioned that he plans to mention to the mid-IR instrument manufacturers that they should include multiple regression math in their software packages - looks like we're getting into the big leagues.

I talked with Sammy Gabriel about his experiences with the I/A 500. Unfortunately we seem to have lost Sammy: he loves the 400's but has given up on trying to make the 500 work and transfer calibrations from it; he can't afford to take a chance on wasting any more time with it.

Jim P. and Apps group: Re the Schiller samples: Karl Norris has run them (grinding on a Udy with no screen), and gotten some interesting results.

He finds no "particle size effect" on the gluten strength measurement with this grinding technique. Phil Williams will measure the actual particle size distributions in Karl's samples. He wants the results of our handling the samples in the standard way. In addition to the standard statistics, he would like us to send him the means and S.D.'s of the samples at 2100 nm and at 1680 nm. He would like these statistics for the hard wheats and soft wheats separately. He would also like us to retain the samples.

Bill Hrushka is also planning to try calibrating using reconstructed spectra, if he ever gets the time. I would love to be able to compare results with him.

Steve J - I think this came up already, but just in case: There is a bug in Data Manipulation - if there is no constituent in a data file (i.e.: DC-type file) then you can't edit the sample number.

Franc Grum (see above) has just set up a Reflectance Standards Laboratory at Rochester Institute of Technology. Mainly he works in the visible and silicon region of the IR. NBS can be expected to move away from standard-setting in the reflectance sciences; non-governmental laboratories will take up the slack. Such laboratories could work toward generating the types of standards we (i.e., the NIRA community) need, but it would be up to us to persuade them of our needs, and provide funding for studies in making such standards. He recommended that we join CORM (Committee On Radiation Measurements), as this organization could help if we can apply our influence to persuade them to meet our needs. Karl Norris plans to become active in CORM; but feels the instrument companies should also join.

Don B.: I received comments on our talk: as I was afraid of, the description of how we generated the design confused people: in the future we would be better off just presenting the design, and emphasize the balanced aspect of it. We should go into the how only if asked.

The session on standards and terminology concentrated mostly on the question of whether NIRA was really a non-destructive procedure; and on the question of defining and measuring "specular" and "Fresnel" vs "diffuse" reflectance. Peter Griffiths offered to be a clearinghouse for discussion on the second question. Bill Hrushka is compiling an exhaustive list of terms that he will include in his chapter in Phil William's book (I'm not supposed to call it that, but it's hard to think of another name for it.)

Tom B., Apps group and Steve J.: On the question of users not skewing up a calibration properly due to poor distribution of samples in the set to be used for measuring the skew: the solution to this problem is to generate two t-values, corresponding to the two null hypotheses: A) that the skew equals unity and B) that the skew equals zero. This is almost trivial to program. However, I suggested that we generate suitable nomenclature for these two hypothesis tests; Dave Hopkins (Dickey-John) Janet Casciero (Pacific Scientific) and myself formed a self-appointed task group to come up with suitable names for these two statistics and send them to Bill for inclusion in his chapter. With luck, this could be the start of having the instrument companies cooperate where it is to our mutual advantage. Creating standards for an industry is beneficial in reducing confusion among the users; increasing the potential market for all companies. Getting a piece of a bigger-pie is better than trying to grab the crumbs of a smaller one. Does anyone have ideas for NEUTRAL names for these two statistics?

Harald Martens proposed a new statistic for indicating the

accuracy of an instrumental measurement, called the Relative accuracy of Prediction; it has several advantages and I want to recommend it, unfortunately I can't read the equation as copied. I will ask Harald for it again, but I would like to be able to give him the info on the ridge regression at the same time: it becomes rather awkward otherwise.

One of the exhibits was an Apple computer based color graphics display where the performance of all possible pairs of wavelengths are displayed as different colors. This makes the nature of the performance characteristics of the various wavelengths choices visible to the user. Despite its limitations it is a very impressive display. (See attached reprint copy - I have the original reprint in color)

## CONCLUSIONS

Since Ron Moen left, Pacific Scientific has nobody of scientific stature except Tom Nolan (maybe this new guy, Pat Cooper, but I don't know him.) Tom is outnumbered: all we need is the will and we can blow them out of the water scientifically - we have the people with the expertise to do it. I think now is a particularly propitious time to start, because we can build on what happened at Chambersburg - we really came out looking good. Particularly the guys in the Apps group can make good contributions to the field in terms of sample handling, which is an aspect of NIRA that is hardly ever discussed. I was able to lay some groundwork for this during our NIRA symposium, and the guys can develop a scientific reputation for themselves if they are so inclined, in addition.