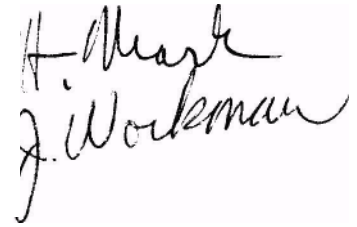


TECHNICON INTERNAL MEMO copy: M. Dzwinczyk

From: H. Mark, J. Workman
To: P. Rotolo
Date: August 25, 1986
Subject: Trip report, Chambersburg
meeting

B. Grusko
R. Rachlis
T. Byron
S. Jackson
C. Kradjel
R. Weedon
D. Burns
G. Kemeny
R. Weiss



Scientifically, the meeting was very fine; people are starting to do hard, serious thinking about the problems of the technology rather than throwing the data into a computer and scratching their heads saying "Gee, I wonder what THAT means?" when the results come out. Also, Technicon put on a very good face, which was appreciated. In fact, Woody Barton thanked us, as Technicon's representatives, for Technicon not sending sales/marketing people to commercialize the meeting.

As important as what was there, perhaps, (but not as obvious) was what wasn't: neither Karl Norris or Phil Williams presented any papers.

Something we noticed on a Pacific Sci. slide was the fact that they offer a computerized bulletin board service for their customers. It seems to us that we should also have something like this. Hardware/software packages for this purpose are available and, once set up, requires very little attention. This seems to be a particularly apropos time to consider this, as we could poll our customers at the upcoming symposium/user's group as to their feeling whether they would actually use this service, were we to provide it.

In addition to the PSCo Bulletin Board, Pacific Sci. is marketing software from InfraSoft Intl. (nutritional and forage), Honigs Scientific Ltd., and Fred McClure(FT-NIR). They also have spectral matching software, which is capable of matching unknown spectra to a spectral library file. Versions of spectral matching software currently under development may be used for quantitative analysis using a library of spectra as known comparison samples. Because of this potential capability we strongly suggest that Discriminant Analysis be expanded by Steve Jackson to be capable of handling more than 100 groups for calibration when he transfers it to the PC.

We recommend that you consider hiring Mark Westerhaus (currently working for John Shenk of Penn State Univ) for the opening for a programming-type in I/A Applications. His address is:

Department of Agronomy
Penn State Univ
13 Pasture Lab
University Park, Pa. 16802
814-863-0779

Miscellaneous facts which may or may not be of interest:

We received a request/idea that Infranet should have the capability of printing out the equations uploaded from a instrument (this would be automatic if we implement the capability of saving an uploaded equation in an equation file).

Karl Norris is measuring wheat hardness by dropping individual grains into a grinder and measuring the acoustic signal as it is ground. However, he and Phil Williams had a long discussion on the meaning of hardness measured this way and whether it or any other measure of hardness was in fact related to the milling and baking properties of wheat.

Lois Weyer, using a Guided Wave instrument to measure a process stream with fiber optics, reported the following standard errors, even though she had 4 mabs noise due to optical losses:

Moisture	.27
Isopropanol	.37
Methanol	.34

Note, what we have been saying for some time is that NIRA accuracy (as defined by RMSD between laboratory procedures and NIR instruments) is nearly always neither instrument noise or math treatment sensitive. Calibration accuracy depends mainly upon sampling and laboratory error considerations. These error sources comprise up to 90% of the total error. We note that Lois' noise levels were 10-20 times those of an InfraLyzer 450, yet SEPs are comparable to those using standard instrumentation and procedures.

Cost of the on-line system is \$20K for the Guided Wave optical box, \$45K for a multiplex system, and \$9/foot for the low-OH fiber cabling. Hercules linked the instrument signal to existing InfraSoft (Shenk and Westerhaus) software on an IBM-pc. Cooled germanium detectors are being used at 200-1600 nm. Fiber optic probes are reported to be robust and capable of withstanding temperatures of less than or equal to 300 deg C and pressures of 5000 p.s.i.

Don Webster reported on the improvements in tilting filters obtainable from using slit illumination, which are considerable compared to keeping the optical beam circular. Pacific Sci also has a fiber optic attachment that uses an annular fiber bundle (collecting fibers surround the illumination fibers) that they used to show an impressive application: simply by pressing it up against your skin, you can measure the body fat content. They say it shows good results compared with other methods of doing this. You can see the fat peak in the spectrum rather clearly. Use of slit illumination has brought about the possibility of greater success in calibration transfer between PSCo monochromators to

PSCo tilting filter instruments.

Keith Snail of the Naval Research Lab described a Compound Elliptic Concentrator, an optical device that can be used in conjunction with integrating spheres to improve their results. He also pointed out that the device can be made in parabolic and hyperbolic configurations also, to be used in appropriate circumstances. Keith introduced several concepts relating to nonimaging optics and the CEC/Sphere template design previously discussed. Certainly, this work may be useful in the development of a generation of InfraAlyzers.

Bob Rosenthal claimed sales of 2000 units (not clear if annual or total figure). He claims applications are: whole pistachio nuts, licorice twists, caramel; all done in transmission. He claimed that 4000 instruments have been sold for transmission measurements in mid and near-IR during the past 4 years. Whole grain can be analyzed by transmission as well flour and milk.

Mark Westerhaus of Penn. State introduced a procedure for correcting calibrations during transfer which showed improved performance over the usual bias and skew procedures. In his suggested method, the individual terms in the equation are corrected using the spectral area immediately surrounding a single wavelength related to each of the coefficients. The procedure involves the calculation of a bias and slope term at each coefficient and makes the correction at each term. The "correction" sample set may be different from the calibration set but it must contain the widest possible range of spectral types.

Isaac Landa made a presentation of his instrument, which can use reflectance, transmission, or fiber optics. He uses a 3M chemometrics software package (SpectraMetrix-TM), for which he has exclusive worldwide license. He claimed all capabilities that we have, and more but the system he had running at the show "didn't have all of them on it" so it is not clear how much of his claims are vaporware. The Landa Rapid Scan Analyzer, termed the Quantum 1200-TM is a grating monochromator capable of operating in 3 ranges (i.e. 400-800 nm, 600-1200 nm, and 1200-2400 nm). The SpectraMetrix-TM software is available for the IBM-PC/AT/XT and consists of a color graphics, window driven, user expandable, MS/DOS system. The menu contains such mathematical capabilities as stepwise regression, factor analysis, and discriminant analysis. A variety of math pre-treatments were claimed to be available including: log 1/R, 1st and 2nd derivatives, derivative ratios, smoothing, ln 1/X, normalization, and Kubelka-Munk. The system uses 0-45 illumination and claims are made that 5 complete scans per second are possible. Isaac demonstrated a complete scan, data transform, and prediction result in 6 seconds total-from start to finish. This same operation requires nearly 2 minutes and three separate operations on our IA 500 with IDAS

software.

Bob Windham (USDA Athens) has done a good deal of work comparing different methods of measuring moisture and concluded that Karl Fisher is the best method to use for the reference method for forage. Not only does the K-F moisture procedure apply to forages, but also to any materials with high volatiles content. Any oil bearing products when oven dried will result in volatile material losses reported as moisture loss. Low and high volatile concentrations within a sample set bring about the addition of stochastic error into the value of Y for calibrations. The addition of this random variability in a calibration set cannot be accommodated by using mathematical techniques.

It has been found that calibration sets can be synthetically generated by moisture addition in products which naturally undergo exposure to moisture and drying. Adding moisture to grain materials to create synthetic calibrations was not found acceptable, possibly due to the "recrystallization" of starch after repeated wet/dry cycles. The moisture in grain does not look exactly like moisture in forages as there are band shifts observable at both the 1445 and 1940 nm regions.

Steve Buco, a statistician who works with Joe Montalvo, has developed a statistic for selecting wavelengths from small sample sets (same one Joe presented at Rocky Mountain Conference). For single-wavelength calibrations using first-derivative mathematics, he finds that the bandwidth over which the Spearman's correlation coefficient of the single-wavelength data is greater than 0.8 is a good indicator. He has done a thorough and correct job of determining this, at least for the type of products their group is concerned with. Limitations of this technique are that the behavior of the algorithm for other types of products is unknown, particularly for cases in which the important bands of the constituent of interest are narrow. Copies of Steve's program are available for SAS in Basic and can be obtained by writing to him.

Ian Cowe presented a paper on principal component analysis (PCA), an area he has worked and published in for some time. His software for use with NIR instrumentation will soon be in the public domain using MS/DOS. PCA is widely discussed and there are several individuals interested in doing further work with the technique.

L. Carriera of the Univ. of Ga. gave a presentation on FTIR. He and Peter Griffiths know each other well, so he must be a mayven in that field. He was also demonstrating a chemometrics package based on FTIR techniques, including Fourier self-deconvolution; a technique that may have merit for our use. His package, or at least part of it, is in the public domain. Carriera's color graphics (IBM-pc compatible), UGA software

includes Fourier or Savitzky-Golay smoothing, Fourier self-deconvolution (mentioned above), differentiation, and integration. The use of FT for database storage space reduction will reduce the required space to store spectra by a factor of 100. The UGA software can be used with very noisy spectra (Fourier smoothing) or can be used to construct a spectrum from the individual component spectra, as well as deconvolve individual absorption bands from overlapped bands. The software uses a binary data format. Conversations related to Carrier's work indicate that he may become one of the very important players in the future of NIR data interpretation.

Looking at this software, as well as other software seen at shows leads to some recommendations for our PC package with color: first, on the spectral plots, when the cursor is turned on, a window should open with a different background color than the main display background and the ordinate and abscissa values presented in this window. When several spectra are displayed, each should be a different color. Digilab has a neat routine that uses a joystick, pushing it up and down expands and contracts the wavelength scale; left and right scrolls through the spectrum; this would be a neat pizzazz feature to have.

Both Lois Weyer and George Anderson found an interesting phenomenon: at least one selected wavelength had zero correlation with the constituent under analysis. This is extremely interesting, because a wavelength with that property would be expected to give optimum correction for an interference.

Tony Davies announced an Analytical Spectroscopy meeting in Norwich July 12-15, 1987 (brochure attached- note Ed Stark on the program).

Jim deHaseth has a mid-IR spectral library search based on doing a dot-product of the unknown against each library entry. This is similar to the discriminant analysis scheme Pacific Sci uses.

Phil Williams thinks he has a scheme for identifying wheat varieties: he extracts the wheat with alcohol, drops the extract onto a fiberglass pad and measures the spectrum. His work so far shows major differences between the different varieties. He would like to use discriminant analysis but, since he doesn't have software, would like to collaborate with us. He proposes to do the lab work and data collection, then send the data in for analysis. The advantages to Technicon are that we would have the only system for discriminating wheat varieties, and we would have a consumable (the fiberglass pads) to sell. However, since he has only Pacific equipment, if we decide to go ahead with this, it would be in our interest to lend him an instrument as well, so that it is clear that only Technicon equipment will be considered suitable for that analysis. We would also publish the work as a

joint paper, to disseminate the information.

Peter Griffiths expects to get a grant to convert his interferometer to a step-drive so that he can do photoacoustic FTIR with it.

Ed Stark is working on determining the optimum point for switching between transmission and transfectance, when analyzing scattering samples. This is an extension of his work on the Halon-oil-Freon mixtures he did, except that he is now doing it for Pacific.

Richard Whitfield (Upjohn) and George Anderson (Pillsbury) both reported on using Mahalanobis distance measurements to determine whether analytical sample belongs to same population as calibration set. Whitfield in particular did a good job of testing the algorithm for this purpose under different conditions.

Other noteworthy events included Gabor Kemeny's paper regarding on-line NIR and Acousto-Optical Tunable Filters and J. Workman's paper on New approaches to forage analysis. H. Mark also attracted favorable attention when presenting "A Day in the Life of a Technicon Applications Scientist."

Mary Cook of Perkin-Elmer discussed their Master Lab System-TM involving robotic sampling, sample identification, sample preparation, and analysis features. P-E's robot is IBM-PC controlled. The complete robotics package for custom applications consists of: (1) the system controller (IBM-PC/AT/XT or Epson Equity), (2) the robot hardware, (3) the sample ID module, (4) the sample preparation module, and (5) the sample analysis module. P-E feels that sample grinding automation is nearly perfected.

The "back to basics" session at the meeting involved papers by Ed Stark, Ian Murray, K. Kaffka, and John Shenk. Each paper addressed the various characteristics of water in the NIR region. Thus, NIR researchers are starting to look at the real chemistry on a well known material- water.

Bill Hruschka presented his paper suggesting that 30 equally spaced wavelengths utilized across the NIR region can be used to generate any closed population calibration equations. This procedure requires very little computational time (30 seconds).

Fran Dennis of Masonite Corp. showed success in calibrating a Pacific Sci. system for in-process on-line analysis of %size in pressed wood panels.

Jon Perkins of Univ. of Wash, presented the mathematics involved in the LaPlace transform spectrometer.

Fred McClure was elected the organizer for the next Chambersburg conference.