

TECHNICON Internal Memo

Date: Aug. 27, 1986.

To: Ms. R. Weiss

From: Dr. G. Kemeny

Subject: Chambersburg Meeting, '86.

Having delayed my report by a few days I received the other trip reports (Dr. H. Mark+Dr. J. Workman and Dr. D. Burns) thus I try to avoid repeating what was already mentioned, as I mostly agree with their content. Consequently it is not necessary for me to go through the list of speakers, below I grouped the information and my impressions according to 5 topics.

1. Technicon is on the defensive in the NIRA scientific community

P. Griffiths (U. California, Riverside) received a Neotec scanning instrument (probably free) and is moving into NIRA. He is a key figure in infrared and FTIR spectroscopy and therefore his decisions and actions are very visible in the whole professional community. I asked if he would be willing to consult for us and he did not exclude this as a possibility.

The "Council for Near-Infrared Spectroscopy" put forward by Ed Stark and voted into existence according to the Constitution will no doubt play a major role in the NIR field. Many fear, and it may not be unfounded, the Council will try to monopolize the future conferences, will try to act as an "official organ" to propose sessions and select speakers. Needless to say that none of the officers are affiliated with Technicon. None of us was invited to take part in the first session on the long list of names but it was however open to the public. So far the next Chambersburg Meeting will not be under the supervision of the council and the Near Infrared Journal (the official publication of the Council) will not contain scientific papers only society news and comments.

Established names are associated with and used by Neotec offering their third party SW giving the impression that they are on Neotec's side (Honigs Scientific - D. Honigs, Infrasoftware-Mark Westerhaus, Penn State, McClure - N. C. State)

2- The new instruments are not better but fancier, but this may prove to be just as detrimental to our position and sales.

Isaac Landa demonstrated his new multipurpose grating

instrument, the Quantum 1200. Some features:

5 full scans/sec (UV-VIS-NIR options)

Solid sample holder or fiber optic (0/45) head

(no mention of liquid cell so far)

Fiber optic cross section about 2 mm x 12 mm (matching the exit slit of monochromator), length about 3 feet. 4 10x10 PbS detectors in head, no collection optics

Has NEMA cabinet version for industrial purposes

LT Industries has about 10 people. An unnamed instrument distributor company from NJ sent their man (R. Rubin) to watch people's reactions to decide to distribute the Quantum 1200 nationwide.

The SW package running on the color PC was written by Landa's men except the stepwise regression, which was licensed from 3M. A copy costs 4K, the basic instrument sells for 38K (but "prices come down dramatically if more units are purchased").

TREBOR sold several hundred units in Brazil for human food applications (school lunch programs). They have a shiny color PC package, and a new scanning (grating) model, the Mod. 7000.

3. NIRA (or NIRS) is maturing in many cases basic spectroscopic principles emerge.

P. Griffiths claims that Kubelka--Munk transformation (first published in 1931) is the real thing, especially if one has to do quantification without prior calibration (his coal oxidation studies). Other manufacturers have K-M (e.g. LT Industries) we should also offer it among other math. transforms on our list. Although it should be tested, generally it is linear in the medium concentration range, and as a continuum model it is theoretically correct only for infinitely small particles.

New techniques are suggested to be borrowed from "other regions of the spectrum". Fourier self-deconvolution can help find and resolve overlapping bands (L. Carreira - U. Georgia). This is another candidate on the long software wishlist for the 500.

4. On-line

In my interpretation the presentation from the Masonote Corp. was not a Neotec success-story. After O.K. lab-calibration and acceptable in-plant calibration adjustment the instrument drifted (oil and moisture content in a 60 % water containing pulp-sheet) and is not used any more.

Hercules Chemical Corp. (Wilmington, Delaware) is experimenting with Guided Wave and Neotec on-line equipment, but is willing to test and evaluate any new, upcoming on-line instrument.

ICI Research Center (also Wilmington, Delaware, Dr. Paul Grady) is ready to discuss their on-line problems, requirements and applications. This makes Wilmington an attractive site for an information gathering tour for on-line development.

To illustrate the harsh environment for on-line instruments: Henkel Corp., Kankakee, IL phased out a Foxboro Infrared process analyzer, which was totally corroded inside in spite of the

nitrogen purging of the instrument house. (NH3 and other corrosive gases in the atmosphere)

General Foods is using the TREBOR instrument (probably the Mod.1000) for on-line QC of rice products. Accuracy and calibration checked 2x/week.

The Quantum 1200 utilizes a programmable bit pattern interface as a coupling to the auxiliary process control equipment.

K. Norris is experimenting (according to some indirect information) with very broad band filters. With 5 filters of about 300 nm bandwidth, covering the whole region it was possible to obtain relatively good calibrations. In a sense this is similar to T. Hirschfeld's plastic filters, that he presented at FACSS '85. I see potential in the use of such filters in some on-line applications (use of fiber optics or remote non-contact optical head), where the low signal energy level would be a source of higher standard error.

After some preliminary studies Cargill, Minneapolis, MN (R. Benson) is probably buying 6 on-line systems from Neotec (Mod. 7000). for various liquid process lines.

G. Anderson (Pillsbury) pointed out that for non-NIRA-insiders the technology loses its image and credibility if a sample can be analyzed and evaluated with the wrong calibration resulting in bad, sometimes negative concentration values. This has to be, and can be avoided by a simple pattern recognition routine which would refuse to provide wrong answer if the sample is outside the reflectance range of samples for which it was calibrated. This feature is advantageous in a lab. instrument but would be a necessity in an on-line analyzer not to shut down the process due to a bad sample or due to a discontinuity in the material flow.

5. Other topics, worth mentioning for their negative merits, are:

Invention of the one_wavelength_moisture_calibration (W. Windham)

Use of fourth_derivative_transformation (J. Shenk)

60-term_calibration (W. Hrushka)

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