

TECHNICON INDUSTRIAL SYSTEMS
Interoffice Correspondence

Date: Aug. 24, 1986
To: B Grusko
From: D A Burns
Subject: 3rd Int'l Diffuse Reflectance Conference

Copy: T Byron RB Roy
G. Kemeny R Weedon
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The meeting last week in Chambersburg PA was very worth while. Technicon had 5 representatives: H Mark, J Workman, T Byron, G Kemeny, & me. R B Roy attended long enough to substitute for R Weedon, and Bob Hertel set up the hospitality suite (which was very well received, and was maintained after he left by T Byron & the others in attendance). There were about 95 registered, including the other instrument manufacturers (all of whom had exhibits). This report includes the technical program, the exhibits, and E Stark's meeting on the Council for NIR Spectroscopy.

Ed Stark organized and chaired the opening session on "Instrumentation" Technicon was conspicuous by its absence; Ed apparently elected to handle it that way. Lois Weyer described her activities with Guided Wave's NIR fiber optic probe, and admitted to its high noise (4000 uA at zero OD) and cost (\$20~45K with 200' fiber). It was used to monitor a liquid stream (carrying the ternary mixture MeQH/IPA/Water) once every 24 seconds. Don Webster talked about Neotec's tilting filters and current work with fiber optics, suggesting on-line capability. Others who described their activities included Keith Snail (Naval Res Lab, work with non-imaging optics). Tony Davies (Norwich Lab, UK, water det'n & noise from air conditioning). Mark Westerhaus (software company with John Shenk, wavelength shift & photometric response), and Pat Cooper (software from Honigs Scientific Ltd, Pacific Scientific's computer bulletin board, and Neotec's interaction with Fred McClure). The session concluded with a commercial pitch by Trebor's Bob Rosenthal (he's pushing for more transmission measurements) and LT's Isaac Landa, who will become stiff competition! Isaac had a nice demo, and described his work with fiber-optics, on-line measurements, rapid scan (including the visible region), 3M's chemometrics, his IBM-compatibility, his use of SpectraMetrix MS-DOS operating system which is "user expandable", his system's cascading capability (we need this!), and his built-in system checks (152 prior to running, and 20 while running). I'm else we didn't have a system sitting alone side his.

Phil Williams organized & chaired the 2nd session. All I heard was Randy Wehling's discussion of automation (lab & on-line, including sample prep, data handling, and control charts) and Chas Shoemaker's presentation of the hazards of data acquisition.

Karl Norris ran the 3rd session in which Ed Stark introduced the subject (moisture) and the others Ian Murray, Karoly Kaffka, John Shenk, & Bill Windham elaborated in considerable detail.

Fred McClure ran the data processing session. Steve Bucu gave essentially the same paper that his co-author Joe Montalvo gave at the Rocky Mt Conference 2 weeks ago, in which he introduced a new statistic based upon peak width; the program MAY be available to anyone. Tony Davies described CARNAC (Comparison Analysis using Restructured NIR And Constituent data) and the "similarity index". Up to and including this paper, I noted that no one had mentioned Technicon equipment, nearly every piece of work had been done with Neotec instruments! Ian Cowe talked about principal components as an alternate data treatment, then Bill Hrushka concluded the session with absorption-based spectroscopy of forages.

Don Webster had a full session which began with Peter Griffiths who addressed the relative merits of Kubelka-Munk and log I/R. There was some question, though, about his use of NaCl as a reference (?), Lois Weyer spoke again (not much new), then Rob Taylor (on textiles). R B Roy discussed NIRA for polymers, then Upjohn's Dick Whitfield described our discriminant analysis program for pharmaceuticals. Pat Cooper ended the session with a talk on "Evaluation of Motor Oil Viscosity* based upon work with Honigs at Univ of Wash (& possibly CPAC).

Carreira's Wed evening session on automated spectral interpretation involved Jim DeHaseth who addressed (1) spectral searching, and (2) structure elucidation. It began with peak tables, then examined compressed spectra, then full spectra, and concluded with Fourier domain searching. Next, Shenk & Westerhaus formed a tag team & went into great detail on the effects of mid-IR bands in the NIR region, using polystyrene as an example. Woody Barton ended the session with the warning that "old technology with a computer merely lets us get wrong answers faster." He's right, of course.

My Thursday morning session ran its full allotted time, with good discussions following each paper. Jerry Workman spoke on "New Techniques for NIRA Evaluation of Forage Quality", and John Diffie (R J Reynolds) described "NIR Calibration Transfer from Neotec 6350 to Technicon 400." John was urged to publish this work ASAP, and he said it was being cleared now. Pillsbury's George Andersen talked about "NIR Analysis of vital Wheat Gluten" and Pat Cooper ended the session with a short talk on "NIR Transmission Spectroscopy for the Analysis of Edible Oils."

That evening we heard Tony Davies again (on JBJ Fourier), Fred McClure with his usual FT/NIR talk, Paul Vane's rather confused and difficult-to-understand mystery hour involving, polarized light, and John Ferraro's talk which covered IR from far, thru mid, to near.

Friday's final session by Dave Wetzel included his own talk on on-line InfraAlyzer work he's done at Kansas State, Gabor Kemeny's description of the acousto-optical tunable filter and its potential, Jonathan Perkins' story on the Laplace transform instrument at Univ of Wash, and Peter Griffiths' interesting talk involving curve fitting, surface chemistry for trace levels (?), S/N ratios, angular dependence of diffuse reflectance, and the evils of using polarizers in diffuse reflectance instruments.

Tony Davies made a strong pitch for 'The First Int'l NIR Spectroscopy Conference' in Norwich, UK, in July 1987. Unfortunately, the speakers have already been selected (by some committee including Stark & several from Europe), so solicitations are for poster sessions only.

On Monday afternoon about 20 people gathered to firm up the constitution for "The Council for NIR Spectroscopy" and elect officers. Not surprisingly, Stark is president, Karl Norris is VP, Fred McClure is sec'y, and Pat Cooper is treas. I'm on the governing board, for whatever that's worth. Dues were established at \$25 for individuals and \$250 for sponsors (which includes two members). We'll be getting a bill, and must decide on the extent of our participation.

The next meeting of this group will be in 2 years, same location.

