

Seventh IDRC Conference – 1994

Chairman: Phil Williams



Phil Williams, (Conference Convener, IDRC VII)

By the time of IDRC VI (Bob Taylor's) the IDRC conferences had matured to the extent that they were attended by upwards of 150 people. Thursday afternoon was allocated to sports (Fred had initiated the PYOT at least two meetings earlier, Art Springstein won the golf every time and Peter Perten spent years trying to beat Bob Taylor – later I golfed with Peter and found that his golf was way better than mine (but a 90-year old cripple with only one hand would have a better handicap than me!), but his golf-cart driving was even worse!) and Thursday evening heralded the conference banquet. The convener of the next IDRC was by then elected by the membership, and of those who had offered to take it on I was surprised when Woody announced at the banquet that I would be convener of IDRC VII. Surprised and pleased, because a couple of years earlier we had invited the NIRS World to Montréal for the 1995 International NIRS Congress, so organizing IDRC VII was good practice for Debbie Sobering (my right hand) and me.

By then the glamorous Kathy Lehman had been Conference Coordinator for the past few meetings, and a joy to work with. At the Sunday evening welcoming session Mayor Robert Morris gave us a glimpse of the influence of the formidable 'flu virus on history. He mentioned that the general who was in charge of one of the armies had indeed planned on setting up camp at Chambersburg, but because of a dose of 'flu the army had to settle for Gettysburg, which in the end of course saved President Lincoln about another day of travel.

The scientific content of IDRC VII was as stimulating as ever. Clinical applications of NIRS were well established. Claus Borggaard gave the first presentation of Artificial Neural Networks at an IDRC (but the ever-innovative Fred had introduced us to ANN at Aberdeen in 1991). Claus predicted that "neural nets" were here to stay, and indeed a few years later Tecator offered ANN calibrations for prediction of protein in, not only whole wheats of different classes, but different types of whole grain, all with the same calibration. An all-grain calibration was also available for prediction of moisture. These have become the mainstay of wheat handling and marketing world-wide. Oh, there were other talks, about things like instrumentation, NIRS networking, On-line and At-line applications, FTIR and FT-NIR, etc. too, just to keep the other people interested! And a growing number of posters.

But tragedy had struck the IDRC, and even the town of Chambersburg had appeared to be slightly subdued when Debbie and I drove in from Harrisburg on the Saturday afternoon. A year or so before the 1994 conference the North Point Tavern closed its doors, so the Chambersburg group was forced to seek an alternative post-conference center for post-technical session technical discussions. The conference convener quickly identified Dave's Tavern on the main drag, an establishment possibly even more sleazy than the North Point, but just a bit too far away from Wilson College for a walk after the evening sessions.

So IDRC VII became the first conference at which evening receptions were organized. The refreshments were sponsored by several companies, who justly received their accolades during each day. The first (and every subsequent) Sunday night reception was sponsored by NIRSystems (now Foss Analytical), and all of the evening receptions from Monday through Thursday were sponsored by different companies, including "The Consultants" (Emil Ciurczak, David Hopkins and Howie Mark in alphabetical order). These came to be held in Laird Hall, home of the exhibitors and posters, so everybody and everything got lots of exposure at modest cost. The college kitchen have always been most helpful with equipment and ice, and there are always a few stalwarts who have managed to stay erect long enough to help with the late-night clean-up.

Onward and upward. And strength to the arms of the organizers of IDRC XIII.

7th International Diffuse Reflectance Conference

August 14-19, 1994
Wilson College
Chambersburg,
Pennsylvania, PA, USA

CONFERENCE PROGRAM

WELCOME

AUGUST 14: Sunday Evening (7 p.m.)

Chairman: Phil Williams, Grain Research Laboratory, Canadian Grain Commission, Winnipeg, Manitoba, Canada (Phone 204-983-3344, Fax 204-983-0724)

Welcome to Chambersburg
Robert Morris, Mayor
Chambersburg, PA, USA

Welcome to Wilson College
Kathy Lehman, Director of Conferences
Wilson College, Chambersburg, PA, USA

Invited Lecture: Ian Murray
Scottish Agricultural College,
Aberdeen, Scotland

*Diffuse Reflectance
Spectroscopy in Agriculture—A
Future Beyond the Visible*

Informal Reception

NEW AND NOVEL INSTRUMENTATION

AUGUST 15: Monday Morning (8 a.m.)

Chairman: David Hopkins, Consultant, Battle Creek, MI, USA

Opening Remarks and Announcements Phil Williams

A Brief Introduction to Kromoscopic™ Analysis—An Alternative to Spectroscopy
Myron J. Block, Optix, Inc., N. Salem, NH, USA

A Comparison of Single Fiber Probe Designs for Remote Spectroscopic Measurements Susan Foulk, UOP Guided Wave, Eldorado Hills, CA, USA

Spectrometry of Small (Microliter or Micrometer) Samples Quickly David Wetzel and Arnold Eilert, Kansas State University, Manhattan, KS, USA

Supporting More Than 100 GRAINSPEC Users
Ole Rasmussen, Foss Food Technology, Canada, Inc., Brampton, ON, Canada

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Coordinator: P. Williams Treasurer: J. Reeves Posters: D. Honigs Exhibits: J. Reeves
Activities: Golf, Volleyball, Tennis, Swimming, Jogging, Walking and Sightseeing

Novel Sampling Techniques for Liquids *Bengt Sahlin, NIRSystems Inc., Silver Spring, MD, and Karl Norris, Engineering Consultant, Beltsville, MD, USA*

Optical Accessories for Spectroscopy *James Harrick, Harrick Scientific Corp., Ossining, NY, USA*

Anyone Can...! High Speed Diode Array Analysis of Whole Grain *Ed Stark and Karen Luchter, KES Analysis, New York, NY, Jim Psoyka and Wes Shadow, Perten Instruments North America, Inc., Reno, NV, USA*

Look, Dave, No Center Peak FTIR *Bill Fateley, D.O.M., Inc., Manhattan, KS, USA*

As the Sphere Turns—Further Adventures in the Seamy Side of FT-NIR Spectroscopy *Art Springsteen and Trudy Ricker, Labsphere, Inc., North Sutton, NH, USA*

Simple, Dedicated, Near-infrared Sensors for Repetitive Sensing *David Honigs, Katrina, Inc., Hagerstown, MD, USA*

On-line Liquid Sensing Using a Fibre-Coupled Probe, with Reference to the Brewing Industry *Peter Hindle, Infrared Engineering, Ltd., Maldon, Essex, U.K.*

Recent R&D in Acousto-Optic Tunable Filter (AOTF) Devices and Spectroscopic Systems *Xiaolu Wing and Ron Rosemeier, Brimrose Corp., Baltimore, MD, USA*

Miniaturized NIR Analyzers *Robert Rosenthal, Futrex, Inc., Gaithersburg, MD, USA*

MEDICAL AND CLINICAL APPLICATIONS

AUGUST 15: Monday Evening (7 p.m.)

Chairman: Jeff Hall, NIRSystems, Toronto, Ontario, Canada

Developing Rapid Spectroscopic Techniques for Rapid Analysis of Whole Blood *Karl Norris, Consultant, Beltsville, MD, USA*

Biodiagnostic NIR at the NRC *Tony Shaw, S. Kotovich and H. Mantsch, National Research Council, Winnipeg, Manitoba, Canada*

Non-invasive Monitoring of Blood Analytes Using Near-infrared Spectroscopy and Multivariate Analysis *Dave Haaland, M. R. Robinson, E. V. Thomas, E. D. T. Jones, T. L. Robinson and R. P. Eaton, Sandia Corporation, National Laboratories, Rio Grande Medical Laboratories and University of New Mexico School of Medicine, Albuquerque, NM, USA*

NIR Spectroscopic Analysis of Physiologic Fluids *Jeff Hall, NIRSystems, Toronto, Ontario, Canada*

CHEMOMETRICS/NOVEL SOFTWARE

AUGUST 16: Tuesday Morning (8 a.m.)

Chairman: Tony Davies, Norwich NIR Consultancy, Norwich, England, U.K.

Artificial Neural Networks and/or PLS-R/PCR for Calibration in Spectroscopic Applications *Claus Borggaard, Danish Meat Research Institute, Roskilde, Denmark*

3D Displays of Sample Populations *Mark Westerhaus, Infracore International, State College, PA, USA*

(continued on next page)

Optimised Scaling Regression: Theory and Practice Tomas Isaksson, Norwegian Food Research Institute, As, Norway

Principal Component Regression and the PRESS: Extracting the Most Information from your Data Steve Buco, Statistical Resources Inc., Baton Rouge, LA, USA

The Evaluation of Some Calibration Transfer Algorithms Jamie Duckworth, Galactic Industries Corporation, Salem, NH, USA

Analysis of Amino Acids Using Expandable Calibrations Ron Rubinovitz, NIRSystems, Silver Spring, MD, USA

Discussion: *Where is Chemometrics Going and Where Would We Like It to Go?*

AUGUST 16; Afternoon Workshops

1:30 p.m. Multivariate Calibration in Practice

**Chairman: Suzanne Schonkopf, CAMO A/S,
Trondheim, Norway**

A practical demonstration of how to use PLS to develop a calibration model and predict concentrations in new samples from NCR. spectra. We will show and explain how to look for outliers, interpret models, and test model performance. The analysis will be performed by "live" use of The Unscrambler software, with focus on practical use of PLS.

**3:00 p.m. What We Have Learned About NIR
in 50 Years of Combined Experience**

**Chairman: Karl H. Norris, Consultant,
Beltsville, MD, USA**

Karl Norris and Phil Williams will illustrate and explain the things they have learned about sample preparation, data treatments, calibration procedures and spectral interpretation in using NIR to measure the composition and quality factors of a wide range of products. This will be an informal session, open to questions and brief comments by participants.

NIR NETWORKING SYSTEMS

AUGUST 16: Tuesday Evening (7 p.m.)

Chairman: Pierre Dardenne, Ministere de l'Agriculture, Libramont-Chevigny, Belgium

An NIRS Network for Tissue Testing of Turfgrass David York, Karsten Turf, Valencia, PA, USA

Operating and NIRS Forage and Feed Testing Consortium Mark Matteson, Neal Martin and Dan Undersander, University of Minnesota, St. Paul, MN, USA

NIRS Network Procedures and Examples Chris A. Drapcho, Infrasoft International, Port Matilda, PA, USA

Networking Essentials: Multiplexing and Calibration Transfer Isaac Landa, John M. Pope and George Asimopoulos, LT Industries, Rockville, MD, USA

The Use of NIR in Danish Agriculture: (a) Recent Experiences with the National Network-System for Quality Assessment of Grain and Rapeseed; (b) The Introduction of a New NTT-Instrument for Animal Feedstuffs Nils Bo Buchmann, Danish Co-operative Farm Supply, Copenhagen, Denmark

Why Should One Build NIR-Networks? E. Wust, Fachbereich Milch-und Molkereiwirtschaft, Hannover, Germany

Monitoring Performance of NIRS Network in the Feed Compounds Industry Ana Garrido-Varo, Escuela Tecnica Superior de Ingenieros Agronomos y de Montes, Cordoba, Spain

FT INFRARED AND NEAR-INFRARED APPLICATIONS

AUGUST 17: Wednesday Morning (8 a.m.)

Chairman: Gabor Kemeny, Nicolet Instruments Corporation, Madison, WI, USA

Qualitative and Quantitative Analysis Using FT-NIR Analysis Gary Dotzlaw, Bran+Luebbe, Inc., Buffalo Grove, IL, USA

Resin Identification by NIR and Neural Nets M. Kathleen Alam, Suzanne L. Stanton and Gregory A. Hebner, Sandia National Laboratories, Albuquerque, NM, USA

Comparison of NIR FT-Raman and FT-NIR Gabor J. Kemeny, Chris Petty, Margaret Fleischli and Casey Bergman, Nicolet Instrument Corporation, Madison, WI, USA

Ultra Spatially Resolved FT-IR Microscopy with a Synchrotron Light Source David L. Wetzel, Kansas State University, Manhattan, KS, USA

SOFTWARE SHOOTOUT

AUGUST 17: Wednesday Workshop (2 p.m.)

Chairman: Fred McClure, North Carolina State University, Raleigh, NC, USA

The objectives of this session are two-fold: (1) To draw attention to the wide diversity of software available for analyzing spectral data; and (2) to impress on participants, including the audience, the advantages and need for sharing data sets in order to advance NIR technology.

Rules for this event are:

1. All participants must use the data set provided by Fred McClure. You may use other data sets if you wish to illustrate a point or make comparisons; but your results, both qualitatively

and quantitatively, must be based on the data set furnished herewith.

2. You are to make both qualitative (e.g., do all samples fit the data set) and quantitative analyses. Quantitative results should be based on the standard error of prediction (i.e., does your calibration perform well).
3. Use any software package you wish. Use more than one package if you wish.
4. You will have approximately 20 minutes to make your presentation. Prizes will be given for the best in-depth analyses. Decisions of the Judges will be final.

SPECTRAL FEATURES ANALYSIS AND INTERPRETATION

AUGUST 17: Wednesday Evening (7 p.m.)

Chairman: James B. Reeves m, USDA, ARS, RNL, Beltsville, MD, USA

Abnormal Spectra: Causes and Cures Karl Norris, Beltsville, MD, USA

Thermal Wave and Optical Reflectance Mechanisms in Infrared Radiometric Systems Andreas Mandelis, University of Toronto, Toronto, Ontario, Canada

Near versus Mid Infrared Diffuse Reflectance Spectroscopy of Forages James B. Reeves HI, USDA, ARS, Beltsville, MD, USA

Note: The Wednesday night session will end at 9:30 p.m. to allow everybody to read the posters, which will be in Laird Hall.

MAKING NIR WORK IN THE INDUSTRIAL WORLD

AUGUST 18: Thursday Morning (8 a.m.)

Chairman: Paul Brimmer, Eastman Chemical Corporation, Kingsport, TN, USA

Determination of Plasticizer Levels in Tenite Plastics by Near-infrared Spectroscopy Candace Sass, Eastman Chemical Co., Kingsport, TN, USA

Recent Examples of NIR Applications Lois G. Weyer, Hercules, Inc., Wilmington, DE, USA

NIR Analysis of Textile Fibers and Yarns: From Bench-top to On-line James Rodgers' and Subhas Ghosh², ¹The Chemical Group of Monsanto, Cantonment, FL, USA; ²Institute of Textile Technology, Charlottesville, VA, USA

Can You Trust NIR with Your Process? Michael Blackburn, Cargill, Inc., Memphis, TN, USA

Thru-the-Container Process Monitoring of Pharmaceutical Solids and Suspensions Lloyd E. Fox and Mark E. Gerger, The Upjohn Co., Kalamazoo, MI, USA

Near-infrared Analysis of a Pharmaceutical Bioprocess Andrew J. Lange, Merck & Co., Elkton, VA, USA

Calibration Development as a Process, Not an Event Frank A. DeThomas, NIRSystems, Inc., Silver Spring, MD, USA

BANQUET

AUGUST 18: Thursday Evening (7 p.m.)

Speaker: Jeanette Graselli, Director, Research Enhancement, Ohio University, Athens, OH, USA

The Promise of Tomorrow Through Technology

ON-LINE AND AT-LINE APPLICATIONS

AUGUST 19: Friday Morning (8 a.m.)

Chairman: Jerry Workman, Jr., Perkin-Elmer Corporation, Norwalk, CT, USA

Opening Remarks; The Challenges of Making Process Measurements on Scattering Materials Jerry Workman, Jr., Perkin-Elmer Corporation, Norwalk, CT, USA

Process Applications of NIR in the Pharmaceutical Industry Emil Ciurczak, Consultant, Laurel, MD, USA

Application of Near Infrared Spectroscopy and Neural Network Methodology to Biological Processes Ming He, University of Maryland, College Park, MD, USA

Process Applications of SW-NIR in the Chemical/Petrochemical Industry Larry McDermott, Perkin-Elmer Corporation, Norwalk, CT, USA

Practical Industrial NIR Implementation for Reflectance Analysis George Asimopoulos and John Pope, LT Industries, Rockville, MD, USA

Applications of On-line Diffuse Transmission for Dairy Products Dave Honigs, Katrina, Inc., Hagerstown, MD, USA

On-line Process Analysis of Dairy Products by Near-infrared Rob Rubinovitz, NIRSystems, Inc. Silver Spring, MD, USA

POSTER TITLES

Chairman: David Honigs, President, Katrina Inc.,
Hagerstown, MD, USA

*Prediction of Theophylline Release Rate from
Compressed Tablets by Near-infrared Spectroscopy*

John D. Kirsch, David J. Margo and James K. Drennen,
Graduate School of Pharmaceutical Sciences, Duquesne
University, Division of Pharmaceutics, Pittsburgh, PA,
USA

*Neural Network Based NIR Prediction of
Content Uniformity in Individual Intact Tablets*

Nadhamuni G. Nerella, John D. Kirsch and James K.
Drennen, Graduate School of Pharmaceutical Sciences,
Duquesne University, Division of Pharmaceutics,
Pittsburgh, PA, USA

Nutritive Value of Portuguese Feeds J. M. Abreu,
Associate Professor, Institute Superior de Agronomia,
Tabada da Ajuda, Lisboa Codex, Portugal

*Measurement of Corn Processing Characteristics
by NIR Spectroscopy* Randy Wehling, Department
of Food Science and Technology, University of
Nebraska, Lincoln, NE, USA

Wheat Hardness: New Insights Marena Manley,
University of Plymouth, Seale-Hayne, Newton Abbot,
England, U.K.

*Automatic Control of Coagulum Cutting in
Cheese Production Using a Fiber Optic Sensor*

F. A. Payne and Karen Lochte, Department of
Agricultural Engineering, University of Kentucky,
Lexington, KY, USA

Textile Quality Control with FT-NIR Donald E.
Muller, Bran & Luebbe, Inc., Buffalo Grove, IL, USA

Introduction to Kromospectroscopy™ Myron J.
Block, Optix, Inc., N. Salem, NH, USA

There will be a prize of US \$200 for the best poster, sponsored by Katrina Inc.

NOTICE

The winner of the Graduate Student Award to attend the 1994 IDRC Conference, sponsored by the Council for Near Infrared Spectroscopy, is

Jing Lu
Department of Biological Engineering
North Carolina State University