

Eighth IDRC Conference – 1996

Chairman: Jim Reeves III



IDRC FLEXIBILITY AND SURPRISE

I would like to start with the question of running the IDRC. While there has never been a time when a candidate for organizing the IDRC could not be found, it has certainly been true that at times only a single candidate has stepped forward and that many excellent choices are reluctant to do so. I would therefore like to share my thoughts on the matter. I found that being treasurer for the meeting was a great way to prepare. As treasurer for both Bob Taylor and Phil Williams I learned all of the details about Wilson College and also saw some of the problems they encountered and how to avoid them. While for many of you this learning period may not be needed or desired, as someone who had never organized anything close, I found it very helpful. The people at Wilson are excellent and really take care of the organization details at the college. In my case, I had decided on the sessions and chosen the session leaders before leaving Wilson. With Wilson handling most of the logistics, other than the liquid lubricants or $\text{CH}_3\text{CH}_2\text{OH}$, and the session chairs organizing the sessions, the role of meeting chair was not really all that time consuming. Your job is just to see that it all comes together and fill in the potholes that inevitably occur.

The pothole for me, and which shows the **FLEXIBILITY** of the meeting, was that just as I was leaving for Chambersburg on the Friday before the meeting I got a phone call informing me that one of our speakers (Ian Murray) had had a heart attack the day before, but could I arrange to pick up several posters he had. As Ian was to have given two talks, this would have left quite a hole for most meetings, but not for the IDRC. It seems that there are always scientists at the meeting with data and slides available if the opportunity presents itself, and other than the concern for Ian, the meeting never missed a beat. I suspect that the meeting could be run with no pre-organization other than suggested topics with anyone who wishes getting a few moments of fame to speak their piece. With experts available on most any aspect of chemometrics, diffuse reflectance, near- and mid-infrared spectroscopy even the

smallest talk can result in what often seems like an endless discussion (**SURPRISE**). I had tried to organize an unorganized session in which anyone was allowed 5 to 10 minutes to discuss a problem they had encountered. One scientist said he had a few slides on soils, which he could not explain, but didn't really see it of interest. After some arm twisting (not many volunteers actually), he agreed to present his slides. After I think about a 3 minute presentation, there must have been an hour of discussion. While difficult to really plan for, the discussions which occur both in the sessions and often continuing afterwards are what makes this meeting different than any other to me. I have been to Gordon Conferences, after which this meeting was suppose to be modeled, but no where else have I ever encountered so many experts who are willing to discuss subjects freely and give advice and yet always in a calm and friendly manner. Perhaps this is due to the fact that almost everyone has been shown to be wrong at least once or more likely it is a tribute to the people who started the meeting and those that have followed the tradition. Personally, I belief it would be very difficult to recreate the atmosphere that exists at this meeting. That is what the IDRC means to me.

8th International Diffuse Reflectance Conference

August 11th - 16th, 1996

Wilson College

Chambersburg, Pennsylvania, USA

CONFERENCE PROGRAM

WELCOME

AUGUST 11: SUNDAY EVENING (7 p.m.)

Welcome to Chambersburg

Robert Morris
Mayor of Chambersburg, PA

Welcome to Wilson College

Kathy Lehman
Director of Conferences
Wilson College, Chambersburg, PA

Invited Speaker

Karl Norris

***Diffuse Reflectance Spectroscopy:
Where Are We and What Needs to be Done?***

Informal Reception Sponsored by Statistical Resources, Inc.

SELECTED TOPICS

WHERE ARE WE and WHAT IS NEEDED?

AUGUST 12: MONDAY MORNING (8 a.m.)

Chair: Bob Taylor, USDA, Clemson, SC,
USA.

Spectral Interpretation in the NIR.

Ian Murray, Scottish Agricultural College,
Aberdeen, Scotland.

***What are the Limitations of Information Content
for NIR Spectra?*** Tony Davies, Norwich NIR
Consultancy, Norwich, UK.

Spectral Regions and Their Merits.

Peter Griffiths Dept. of Chemistry, Univ. of Idaho,
Moscow, ID, USA.

***Standardization, Calibration Transfer, and
Monitoring.*** Charles R. Hurburgh, Jr., Iowa State
Univ., Ames, 10, USA.

***Where Have We Been and Where Are We Going
in Agriculture.*** Phil Williams, Grain Research Lab.,
Winnipeg, Manitoba, Canada.

AUGUST 12: MONDAY EVENING (7 p.m.)

Chair: Mike Zapf, McCormick & Co.
Inc., Tech. Ctr., Hunt Valley, MD,
USA.

***Recent Experiments in Mid- and Near-Infrared
Spectroscopy.*** David L. Wetzel, Kansas State Univ.,
Manhattan, KS, USA.

***Effects of Ionic and Salt Concentrations on Aqueous
NIR Spectra.*** Emil Ciurczak, Consultant, Laurel,
MD, USA.

***Near-Infrared Analysis of Total Dietary Fiber in
Cereal Products with High-Fat and High-Sugar
Content*** Sandra F. Kays, William R. Windham, and
Franklin E. Barton, II, Russell Research Center,
USDA, Athens, GA, USA.

Looking at PLS Again, For the First Time!
David Hopkins, Consultant, Battle Creek, MI, USA.

***How to Do 200 Calibrations, and Still
Remain Conscious?*** Moise Hoar, LT
Industries, Inc., Rockville, MD, USA.

Informal Reception Sponsored by **David Hopkins**

**WHAT'S NEW IN HARDWARE
AND SOFTWARE?**

AUGUST 13: TUESDAY MORNING (8 a.m.)

Chairs: Howard Mark, Consultant,
Suffern, NY, USA, and Emil
Ciurczak, Consultant, Laurel,
MD, USA.

Presentations of the latest advances in
instrumentation and/or software will be made by
representatives of the following companies:

Bran+Luebbe
Brimrose Corp. of America
Bruker
Galactic Industries Corp.
Kett
LEGO Corp.
LT Industries, Inc.
The Near Infrared
Research Corp.
Perkin Elmer
Perstorp Analytical
Pertten Instruments
SciOptics Corp. (Rep. for CAMO)
Zeltex, Inc.



WHAT'S THE PROBLEM?

AUGUST 13: TUESDAY EVENING (7 p.m.)

Chair: Bob Windham, Russell Research Center,
USDA, Athens, GA, USA.

***Wheat Analysis: New Approaches to Sample
Presentation.*** A. Kettry and J. Psotka, Pertten
Instruments North America, Inc., Reno, NV, USA.

Wet Forage Analysis by NIR. Ian Murray, Scottish
Agricultural College, Aberdeen, Scotland.

How Should We Treat the Data? Karl Norris and
Stephen R. Delwiche, Beltsville, MD, USA.

Analysis of Mixtures of Soil Separates.
Mark Westerhaus, Infracore International, State
College, PA, USA.

***Calibration Transfer Software: A Necessary Tool for
Successful On-Line NIR Analysis.***
Ursula Eschenauer and Stephen V. Medlin,
Brimrose Corp. of America, Baltimore, MD, USA.

Informal Reception Sponsored by

Perkin Elmer

THE "NEW MATH"

SOFTWARE SHOOTOUT

AUGUST 14: WEDNESDAY MORNING (8
a.m.)

Chair: Lois Weyer, Hercules Corp.,
Wilmington, DE, USA.

Feature Selection Using CART. Stephen Sum, Dept.
of Chem. and Biochem., Univ. of Delaware,
Newark, DE, USA.

***Genetic Algorithms as a Tool for Feature Selection
and its Application in NIR.***

Riccardo Leardi, Ins. di Anal, e Tech. Farm, ed
Alimen, Genoa, Italy.

***An Overview of the Wavelet Transform and its
Applications.*** Allan Moser, E.I. Dupont de Nemours
& Co. Inc., Wilmington, DE, USA.

***Rugged NIR Calibrations using Neural Networks
with Comparisons to PLS.*** Paul Gemperline, East
Carolina Univ., Greenville, NC, USA.

AUGUST 14: WEDNESDAY EVENING (7
p.m.)

Chair: Fred McClure, North Carolina State
Univ., Raleigh, NC, USA.

Participants will demonstrate how they analyze NIR
data using the software of their choosing. Two data
sets, one biological and one industrial, were made
available to interested parties. The following victims
have agreed to share their experience with us.

Dianna Jones	SciOptics
Tony Davies	NIR Consultancy
Claus Borggard	Danish Meat Res. Inst.
Susan Foulk	Guided Wave
Jamie Duckworth	Galactic Industries
Bennett Crowell	NC State Univ.
F. E. Barton, II	USDA
David Hopkins	Consultant
Peter Hindle	Infrared Engin. Ltd.
Joe Montalvo	USDA
Alan Moser	E.I. Dupont
Riccardo Leardi	Genoa, Italy

Wrap up: Fred McClure and Lois Weyer. Informal

Reception Sponsored by **Bran+Luebbe**

**NON-NEAR-INFRARED
DIFFUSE REFLECTANCE**

AUGUST 15: THURSDAY MORNING
(8 a.m.)

Chair: Randy Wehling, Univ. of
Nebraska, Lincoln, NE, USA.

Reflectance Measurement and Analysis in Remote Sensing for Agricultural and Natural Resource Applications. Charlie Walthall, RMSL, USDA, Beltsville, MD, USA.

Quantifying What the Eye Can See.
Fred McClure, North Carolina State Univ.,
Raleigh, NC, USA.

Single Beam Substitution Error in Single Beam Integrating Sphere Reflectance Spectroscopy. Art Springsteen, Labsphere, North Sutton, NH, USA.

High Fidelity Raman and Infrared Spectroscopic Imaging.
Linda Kidder, NIH, Bethesda, MD, USA.

Vibrational Spectrometry of Powdered and Rough Bulk Samples: Where Do FT and CCD Raman Fit Into the Picture. Peter Griffiths and Ian R. Lewis, Univ. of Idaho, Moscow, ID, USA.

AUGUST 15: THURSDAY EVENING (7
p.m.)

Pre-Banquet Reception Sponsored by **NIR**

Publications

Speaker: Dr. H. John Wood, Science
Outreach Manager for Hubble
Space Telescope Project, Goddard
Space Flight Center, NASA,
Greenbelt, MD, USA.

Latest Scientific Results from HST

NOVEL APPLICATIONS

AUGUST 16: FRIDAY MORNING (8 a.m.)

Chair: Peter Flinn, Pastoral & Vet. Institute, Hamilton, Australia.

Depth-resolved NIR Spectroscopy. **Jim**

Drennen, Duquesne Univ., School of
Pharmacy, Pittsburgh, PA, USA.

***Near Infrared Spectroscopy for Detection of Water
Content in Two In Vitro Models of Brain Edema.***

Lee Johnson, John Hopkins Univ., School of
Medicine, Baltimore, MD, USA.

NIR Transmittance of Intact Tablets. Bruce
Buchanan, Merck & Co., Inc, USA.

Rapid ID of Plasticizer Levels in Cigarette Filter

Rods. Atul Khettry and J. Psotka, Perten
Instruments, Reno, NV, USA.

***Applications of Near Infrared Spectroscopy in
Environmental Studies.*** Phil Williams, Grain Res.
Lab., Winnipeg, Manitoba, Canada.

On-Line Analysis of Ground Beef. Tom as
Isaksson, Agricultural Univ. of Norway, Dept. of
Food Sci., As, Norway.

***Application of NIR Reflectance for Evaluating Acacia
Timber for Pulping,*** Ian Murray, M. Werren and R.
M. Paterson, Scottish Agric. College, Aberdeen,
Scotland.

***Can NIR Help Save An Endangered Australian
Cockatoo?*** Graeme Batten, Yanco Agricultural Inst.,
Yanco, Australia.

POSTERS

Chairs: Carol Kennedy, Pro Form Feeds, Chilliwack, BC, Canada, and David Ryan, Central Soya Inc., Ft. Wayne, IN, USA.

Poster presenters will be with their posters from 1:30 to 3:30 on Tuesday, refreshments will be available.

Classification of Normal and Acceleratedly Aged Seeds by Principal Component Analysis (PCA) of Near Infrared Spectra. Toyoko Kusama, Hideyuki Abe, and Sumio Kawano, National Food Research Institute, Tsukuba, Japan.

Near Infrared Spectroscopy of Oils During Autoxidation With and Without Antioxidants. P. Plew, I. Murray and J. R. Scaife, Scottish Agricultural College, Aberdeen, Scotland.

Absorption Characteristics of Homogenized Beef and Beef Adipose Tissue in Transmission Mode in the Visible and NIR Region. D. Cozzolino, I. Murray and R. Paterson, Scottish Agricultural College, Aberdeen, Scotland.

The Use of Near Infrared Reflectance Spectroscopy to Determine the Mode of Action of Enzyme Additives for Grass Silage. M. L. Swift, M. A. G. Vonkeyserlingk, J. A. Shelford, and R. J. Treacher, Pro Form Feeds Inc., Chilliwack, B. C., Canada.

The Use of Principal Component Analysis/Partial Least Squares Regression in the Interpretation of Near Infrared Application in Cereal Research. P. C. Williams, Grain Research Lab., Winnipeg, Manitoba, Canada.

New Results in Rapid Qualification by Polar Qualification System (PQS). Karoly J. Kaffka, Univ. of Horticulture and Food Industry, Budapest, Hungary.

Effect of Spectral Resolution on NIR Analysis. Qian Wang, Bruker Optics, Billerica, MA, USA.

Identification of Rice Varieties Using Image Processing Technique and NIR Spectroscopy. Rae Kwang Cho, Dept. of Agricultural Chemistry, Kyung-pook National Univ., Taegu, Korea.

Rapid Quality Evaluation of the Hot Bean Paste by NIR Spectroscopy. Rae Kwang Cho, Dept. of Agricultural Chemistry, Kyung-pook National Univ., Taegu, Korea.

Soft X-Ray Imaging for Foreign Materials in Foods Using Image Intensifier Detector. Shigo Miyamoto, Univ. of Georgia, College of Agri. and Env. Sciences, Biol. and Agri. Eng., Drifitmier Engin. Center, Athens, GA, USA.

New Variable Selection Techniques Applied to Near IR Spectra. Lois G. Weyer, Hercules Corp. and Steven D. Brown, Univ. of Delaware, Newark, DE, USA.

Effect of Water and Physical State on Partial Least Squares (PLS) Near- and Mid-Infrared Calibrations for Multi-Component Carbohydrate Mixtures. James B. Reeves, III, NCML, ARS, USDA, Beltsville, MD, USA.

Wax Content of Cotton Using Near-Infrared Reflectance. Robert A. Taylor and Jim Psotka, CQRS, ARS, USDA, Clemson, SC and Perten Instruments, Reno Nevada, USA.

Designing and Testing Backpropagation Networks for Analyzing NIR Data. M. Hana and W. F. McClure, North Carolina State Univ., Raleigh, NC, USA.

The Ratio Derivative Method for Quantitative NIR Analysis. J. Lu and W. F. McClure, North Carolina State Univ., Raleigh, NC, USA, and F. E. Barton and D. S. Himmelsbach, Russell Res. Ctr., ARS, USDA, Athens, GA, USA.

Analyses of Intact Grass Silages by Near-Infrared Reflectance Spectroscopy. C. A. Kennedy, Pro Form Feeds, Chilliwack, BC, Canada, and J. A. Shelford, Univ. of British Columbia, BC, Canada.

NIR Applications In Nylon Industries. Herman He, LT Industries, Rockville, MD, USA.

On-Line Analysis of Hydrogen Peroxide and Water Vapors During Sterilization Using Near Infrared Spectroscopy. Seetha Ananth, Gary Lang, Rosemount Analytical Inc., Orville, OH and David Crozier, Eli Lilly and Co., Indianapolis, IN, USA.

Use of Near-Infrared Reflectance Spectroscopy and Principal Component Analysis as a Tool for Detecting Heavy Metal-Organic Matter Associations. Dianne F. Malley, Phil C. Williams*, Joanne Delaronde and Laurie J. Wesson, Freshwater Institute, Dept. of Fisheries and Oceans, Central and Artic Region, Winnipeg, Canada and *Canadian Grain Commission, Winnipeg, Canada.

NIR Tissue Analysis Improves Yield and Quality of Australian Cereal Crops. V. B. McGrath, A. B. Blakeney and G. D. Batten, Yanco Agricultural Institute, Yanco, Australia.

The Handbook Be Damned!!! We Can Have a Better Theory (of Diffuse Reflectance). Donald J. Dahm, TechMan Enterprises, and Kevin D. Dahm, M.I.T., Dept. of Chem. Engineering, Boston, MA, USA.

Observations On the Influence of Turbidity on NIR Spectra. Gitesh Kumar and Joesph M. Schmidt, Dept. of Electrical and Electronic Engin., Hong Kong Univ. of Science and Technology, Hong Kong.

Non-Destructive Assessment of Kiwifruit Quality Using NIR Spectroscopy. David C. Slaughter, Univ. of Calif., Davis, CA, USA.

Grey Standards. A. M. C. Davies, Norwich Near Infrared Consultancy and M. P. D. Coene, School of Chemical Sciences, Univ. of East Anglia, Norwich, UK.

EXHIBITS

Representatives of the following companies will be on hand exhibiting various hardware and software products used in reflectance spectroscopy.

Brimrose Corp. of America
Council for Near-Infrared Spectroscopy (CNIRS)
Galactic Industries Corp.
Harrick Scientific
LECO Corp.
Perkin Elmer
Perstorp Analytical
Perten Instruments
SciOptics Corp. (Rep. for CAMO)
Zeltex, Inc.

STUDENT AWARD WINNERS

The winners of the student awards sponsored by the Council for Near-Infrared Spectroscopy were:

Gabriella Kisko, University of Horticulture and Food Industry, Budapest, Hungary, and

Gitesh Kumar, Hong Kong University of Science and Technology, Dept. of Electrical and Electronic Eng., Kowloon, Hong Kong.

Congratulations to both of the winners!

GENERAL INFORMATION

Meals each day: Breakfast - 6:45 to 8:00
Lunch - 12:15 to 1:30 (12:00 to 1:30 on Friday).
Dinner - 5:30 to 6:30 (excluding Thursday night banquet).

Sessions: All morning sessions start at 8 a.m. and evening sessions at 7 p.m.

Sunday-Thursday: After the evening session, there will be an informal get together in Laird Hall.

Monday-Thursday: Swimming pool open daily from 1:30 till 4:30 p.m.
Activities including golf, volleyball, and running will be organized.

Tuesday:

Wednesday:

Thursday:

Departures:

Poster presenters will be with their posters from 1:30 to 3:30 p.m., refreshments and snacks will be available.

Change of towels and wash cloths, place dirty linen outside door in the morning for replacements.
Afternoon trip to Gettysburg, sign up sheet on bulletin board near dining room entrance.

Council for Near-Infrared Spectroscopy meeting from 1:00 to 2:00 p.m., location to be determined.

The Council for Near-Infrared Spectroscopy User's group will meet from 2:00 to ?? p.m. location to be determined.

Please sign up for return rides on Friday to the airport of your choice. Sign up sheets for those needing a ride or those able to offer a ride will be on the bulletin board near dining room entrance.

REMEMBER TO TURN IN YOUR ROOM KEY OR YOU WILL BE BILLED.

Messages:

Post on bulletin board near dining room entrance.