

## **Ninth IDRC Conference – 1998**

### **Chairman: Lois Weyer**



### **Some personal notes on the 1998 IDRC**

Lois Weyer

For me, the “Chambersburg” conferences have been a wonderful series of experiences, beginning with my first one in 1984. I have been amazed at the friendliness and support I received at the meetings. I was inspired by the presentations and discussions and encouraged by the interest in my small experience with traditional NIR and band assignments, and some of the chemical applications I had experimented with. I didn’t find the competitiveness that I found at my job among the NIR community, and the encouragement I received from it really helped me.

So, after working up through raising my hand and objecting to a speaker’s statement that “the near IR region has no useful spectral bands that the mid IR doesn’t also have”, to contributing a three-minute applications spot, to presenting a full talk, to chairing a couple of sessions, I agreed to chair the 1998 conference. I had never spoken up in a large meeting before the 1984 event, but I became more and more confident after I attended and spoke at each Chambersburg (and some international) conferences. So, by 1998, I was ready to add my square to the patchwork quilt of the IDRC.

The first time I had checked in, in 1984, Phil Williams said to me, “Great! Another woman registered.” I was a bit leery about why he said that, but I soon found that the reason was the dearth of women working in the field at that time. In spite of us being at a women’s college, I found that some aspects of the conference were not women-friendly. My first-floor dorm room’s curtains didn’t close very well and I had no pillow, everyone stayed up too late and became more and more tired as the week went by, and the shirts were too large and in only one color – a somewhat translucent white.

So, when I had the chance, I made some efforts to gender-neutralize the conference a bit. First, I handed out a questionnaire at the 1996 conference to gather opinions on what others wanted. Then, I shortened the 7-10 PM evening sessions to 7-9 so that we could get a little more sleep. Next, I offered a pre-conference choice of shirt size and color, arranged for a female banquet speaker on art forgery, and organized bus trips to the Hershey chocolate factory, Hershey gardens, and outlet shopping, as well as Gettysburg and the Hershey amusement park. I also planned both introductory and advanced chemometrics courses and an intro NIR course for the weekend before the conference, even though weekend space was tight and I had to go and buy pizzas for the lunches for the course participants.

With the help of great session chairs and many other people, the technical program fell into place and the conference moved along. People still stayed up late, but at least it wasn't my fault. I think that most of the men also enjoyed the Hershey trip, the shirts, and the banquet speaker.

I had an enjoyable time meeting and talking with all those who came, and am grateful to the people who helped me out in various ways. Thank you, all.

**9th International Diffuse Reflectance Conference**

**Sponsored by the Council for Near Infrared Spectroscopy**

**August 7-14, 1998**

**Final Program**

**WELCOME TO CHAMBERSBURG**

Friday, August 7

5:00-10:00 PM - registration for those attending the Saturday short course.

6:30-7:15 - Dinner

Saturday, August 8

Basic NIR short course, Rosenkrans Hall - presented by Tony Davies of the Norwich NIR Consultancy

8-9AM - Breakfast in dining hall

9:00 AM - Short course begins in the lower level of Rosenkrans Hall

10:30 AM - Break, with coffee, tea, pastries and/or donuts

1:00-1:45-Lunch

3:00 - Break, with sodas and snacks

6:30-7:15-Dinner

Registration for Sunday course participants and other Saturday guests is in Rosenkrans Hall. Keys will be distributed from 5-8 PM.

Sunday, August 9

Continuation of basic course, focusing on PCA and PLS calibration techniques in practice, presented by Michael Bystrom of CAMO,

*or*

Advanced topics NIR/chemometrics course, presented by Tom Fearn of University College London. Neural networks will be discussed in the first hour, followed by wavelet transforms and Fourier transforms. In the afternoon, wavelength selection techniques including genetic algorithms and simulated annealing will be covered.

8:00-9:00 - Breakfast for attendees of both courses  
9:00 - PCA/PLS course begins in Norland Hall parlor.  
10:00 - Advanced course begins in Rosenkrans classroom, lower level.  
10:15 - Break for PCA/PLS course  
11:00 - Break for Advanced course  
1:00 - 1:45 - Lunch for both courses  
2:00 - Advanced course reconvenes  
2:15 - Break for PCA/PLS course  
4:00 - Close of both courses  
5:30 - 6:30 - Dinner for all registrants

3:00 -10:00 PM - Conference registration, at the entrance to the dining hall.

7:00 PM Conference Opening, at the Havens Science Center

Invited Speaker - Fred McClure - "Biomeasurements in the 21st Century"

8:30 - 11:00 - Informal reception in Laird Hall

Monday, August 10

8-12: Physics of Diffuse Reflection, chaired by Peter Griffiths of the University of Idaho

Donald Dahm, Kevin Dahm, and Karl Norris, Techman Enterprises - "Improving the Kubelka-Munk Equation, a Theory of Diffuse Reflectance for Spectroscopists, not Physicists"

Eva Sevick-Muraco, Purdue University - "Photon Migration"

Satoru Tsuchikawa, Nagoya University - "Construction of a New Optical Model and Application of Time-Resolved NIR for Biological Materials with Cellular Structure"

David Burns, Magill University - "Quantitative Three-Dimensional Imaging of Absorbing Materials in Scattering Media Using Time-of-Flight Photon Detection and Mathematical Models of Light Propagation"

1 -2: Informal discussion of the theory of diffuse reflection led by Donald Dahm and Thorsten Burger, tentative location is in the board room in Laird Hall

7-9: Sampling/Sample Preparation, chaired by Phil Williams, Canadian Grain Commission

Sue Lister, Institute of Grassland and Environmental Research - "Sampling and Sample Preparation of Forages"

Jeffrey Hall, Foss/NIRSystems - "The Sample Interface: Key to Success in the Industrial Marketplace"

Diane F. Malley, PDK Projects Inc. - "Sampling and Sample Preparation for Environmental Applications of NIR"

Arnold Eilert, Bran + Luebbe - "Sampling Methods for On-Line Spectroscopy"

Tuesday, August 11

8-12: Spectroscopy, Interpretation, Referee Methods, chaired by James Reeves, USDA

Heinz Siesler, University of Essen - "Towards a Better Understanding of the Interpretative Aspects of NIR Spectroscopy"

Venkatesh Iyengar, NIST - "Primary Determinants in Nutritional Metrology"

Douglas Archibald and Sandra Kays, USDA - "Spectral Window Preprocessing for Improved Model Interpretation: Application to NIR Reflectance Analysis of Unground Cereal Food Products"

John Kirsch and Jim Drennan, Duquesne University - "The Effect of Reference Method on the Quality of Near-IR Calibrations for Dosage Form Coatings"

Lois Weyer et al - informal discussion of referee technique problems and solutions

1:30-3:30: Poster presentations in Laird Hall

7-9: Standardization and Calibration Transfer, chaired by Bruce Campbell, Cytec Corp.

Christian Mittermayr, University of Delaware - "Calibration Transfer from the Perspective of Signal Processing and Soft Models"

Eric Bouveresse, University of Genoa - "Guidelines to Select the most Suitable Standardization Approach"

Roland Winzen, University of Essen - "Calibration Transfer Between Extremely Different NIR Spectrometers"

Wednesday, August 12

8-12: Chemometrics, organized by Paul Gemperline, East Carolina University

Howard Mark, The Near Infrared Research Corporation - "Wavelength selection techniques"

Tom Fearn, University College London - "Calibrating with Wavelets"

Barry Levine, Clarkson University - "Innovative Genetic Algorithms"

John Kalivas, Idaho State University - "PLS and PCR - The Same and Not the Same"

Michael J. McShane, Texas A&M University - "Wavelength/Channel/Variable Selection in Spectroscopy"

1-5: Bus trips. Two 47-seat and one 22-seat buses have been rented for the afternoon. One or two buses will travel to the city of Hershey, PA and will leave people off at one of several destinations: 1) Hershey Park, a large, beautiful amusement park with rides, entertainment, and food, 2) Chocolate World, adjacent to the theme park, a visitor center containing a free ride through a mock chocolate factory plus shopping (you can mail Hershey chocolate items all over the world) and food court including Hershey chocolate items, 3) botanical gardens with a new butterfly house, 4) a zoo of North American animals, and 5) a museum of Pennsylvania and Hershey history including migrations and the story of the Amish people. The conference has purchased group rate tickets for \$20 a person (compared to regular admission at \$29.95). A second bus will be traveling to Gettysburg, a Civil War battle site which has many tourist attractions such as simulated battle scenes, tours of houses, etc. You can sign up for a battlefield tour bus when you arrive at Gettysburg and can walk to various locations. Look for sign-up sheets for either trip location on the bulletin board outside the dining hall.

7-9: Instrumentation News, chaired by Howard Mark, The Near Infrared Research Corporation

This session will include short talks from as many vendors as volunteer, to present the latest advances in their instrumentation.

Thursday, August 13

8-12: Software Shootout, chaired by Fred McClure, University of North Carolina

This session will feature both formal and informal participants, presenting their results on a data set which has been provided by Fred McClure and posted on the Council for Near IR Spectroscopy (CNIRS) website. There will be several invited participants, including Marc Meurens of Universite Catholique de Louvain, Karl Norris, Tony Davies, Susan Foulk, and Peter Griffiths.

1-5: Vendor Workshops, including a CAMO demo on classification/calibration, a Bran+Luebbe workshop on their latest software, and an Analect demo. These will be held in Rooms 113,123, and 129 in the Science Center.

1-2: CNIRS Meeting, including planning for IDRC 2000.

6-8:30: Banquet: Speaker- Janice Carlson of the Winterthur Museum, presenting "The Use of Spectroscopy in Uncovering Fraud and Deception in Art and Antiques"

Friday, August 14

8-12: Special Applications, chaired by David Hopkins, Consultant

Karoly Kaffka, University of Horticulture and Food Industry, Budapest - "The Use of the Polar Qualification System (PQS) in NIR Imaging Technology"

Gary Ritchie, Purdue Research Center - "Qualitative Near Infrared Analysis in the Pharmaceutical Sector"

Mark Dombrowski, Surface Optics Corporation - "Real-Time Hyperspectral Imaging: Revealing the Unseen"

Neil Lewis, National Institutes of Health - "Chemical, Biological, and Clinical Applications of Infrared Spectroscopic Imaging"

Mark Brezinski, Cardiac Unit, Knight Catheterization Laboratory - "Imaging Human Disease at or near the Cellular Level with Optical Coherence Tomography"

Posters

"Time-Resolved Near Infrared Spectroscopy and Related Optical Models for Biological Materials," Satoru Tsuchikawa and Shigeaki Tsutsumi, Nagoya University

"Diffuse Reflection Study of Irradiated, Shelf-Aged Ultra-High Molecular Weight Polyethylene Bar Stocks," M. Shah Jahan, Department of Physics, University of Memphis

"A Comparison of Two Methods for Determination of the Effective Sample Size in NIRS, One Empirical and One Based on the Theory of Radiative Transfer," Ola Berntsson, Royal Institute of Technology, Stockholm, Sweden

"Calibration Transfer Techniques," two posters, by Roland Winzen and Michael Horn, Department of Physical Chemistry, University of Essen

"NIRS in Clinical Chemistry," Volker Neumeister, Dresden, Germany

"Mycological Qualification of Hungarian Red Pepper with the Help of NIR Spectroscopy," Gabriella Kisko, University of Horticulture and Food Industry, Budapest

"Near Infrared Spectroscopy of Polymer Mixtures by Diffuse Reflectance," D. Fischer, Institute of Polymer Research, Dresden, Germany

"The Variety of Scattering Effects in Hair and their Origin," Kathleen Martin, Helene Curtis Inc.

"Comparison Between NIR Measurement on Whole and Filleted Salmon," Christel Solberg, Boda College, Norway

"Performance Standards for NIR Analyzers in Consumer or General Textile Operation," Charles Hurburgh, Iowa State University

"NIR Analysis of Residual Moisture in Lyophilized Products," Robert Leasure, Foss/NIRSystems

"NIR Reflectance of Unground Cereal Food Products for Determination of Total Dietary Fiber", Douglas D. Archibald and Sandra E. Kays, USDA

"A Sampling Strategy to Facilitate Measurement of Both NIR Reflectance and Raman Spectra for Determination of Food Constituents", Douglas D. Archibald, David S. Himmelsbach, Sandra E. Kays, and Franklin E. Barton, II, USDA

"A Network of Near-Infrared Units for Coarse Grain Analysis", Charles R. Hurburgh Jr., T. J. Brumm, G. R. Rippe, C. L. Hardy, and H. S. Park, Iowa State University

"Near-Infrared Reflectance Models for the Prediction of Protein in Mixed Grain Cereal Products", Sandra E. Kays, Franklin E. Barton, H, and William R. Windham, USDA

"Direct Calibration transfer Without Chemometric Enhancement," M. Hawkins, Bomem, Inc.

"Wavelet and NIRS for Single Spectrum Mastitis Diagnosis," Dr. Roumiana Tsenkova, Associate Professor, Kobe University Faculty of Agriculture

"Discrete Ordinate Approximation of the Equation of Radiative Transfer to Characterize Disperse Media from Diffuse Reflectance and Transmittance Measurements," T. Burger, J. Kuhn\* and J. Fricke, Universitat Wurzburg, \*Bavarian Center for Applied Energy Research

"Monitoring the Degree of Cook in Extrusion Processes Using NIR,"  
AJ. Evans<sup>1</sup>, S.Huang<sup>1</sup>, A.Htoon<sup>1</sup>, B.G. Osborne<sup>2</sup>, Z. Kotwal<sup>2</sup> and I.J.Wesley<sup>3</sup>  
1 Food Science Australia, 2 BRI Australia Ltd, 3 CSIRO Plant Industry

"Counterfeiters Beware! NIR Can Catch Those Who Would Print Bogus Currency or Manufacture Fake Turquoise," Don Burns, Los Alamos

"Nondestructive determination of geographic origin of ginseng by Near Infrared Spectroscopy/Raman Spectroscopy," Hyo-Jin Kim, Young-Ah Woo, JungHwan Cho, and Hoeil Chung, Department of Pharmacy, Dongduk Women's University

"Nondestructive Determination of Free Acid and Malic Acid Content in Apples using Near-infrared Spectroscopy," Mi-Ryeong Sohn and Rae-Kwang Cho, Department of Agricultural Chemistry, Kyungpook National University, Korea



"Identification of Geographical Origin of Sesame Seeds by Near Infrared Spectroscopy," Young-Kil Kwon and Rae-Kwang Cho, Department of Agricultural Chemistry, Kyungpook National University, KOREA

"Wavelength Selection for NIR Calibration to Determine Fat in Milk Having both Properties of Scattering and Characteristic Absorbing," Sumio Kawano and Chie Iyo, National Food Research Institute, Japan

"Study on NIR Quality Evaluation of Intact Fruits, Limits of Acidity Determination, and Effect of Storage on Sugar Determination," Chie Iyo and Sumio Kawano, National Food Research Institute, Japan, Nondestructive Evaluation Laboratory National Food Research Institute Ministry of Agriculture, Forestry and Fisheries

"Calibration Transfer in FT-NTR Analysis," Basil Desousa, Bruker Optics "Optimizing

Experimental Parameters in NIR," Basil Desousa, Bruker Optics

"Spectral amplification in NIR spectroscopy and sorting of whole apples," Meurens, M. and E. Moons, North Carolina State University

"A Hand-held NIR Meter for Measuring Chlorophyll and Moisture in Plant Materials," McClure, W.F. and D. Stanfield. North Carolina State University

"What is the optimal absorbance in NIR spectroscopy?" Isaksson, T., Segtnan, V.H. and Thyholt, K. Dept. Food Science, Agric. University of Norway

"Representative Layers of Particulate Solids," Donald J. Dahm, TechMan Enterprises.

"NIR imaging spectroscopy of Kiwifruit Slices," Paul Martinsen and Andrew McGlone HortResearch

### **Student Award Winners**

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

Thorsten Burger, University of Wuerzburg, Germany

Ola Berntsson, Royal Institute of Technology, Stockholm, Sweden

**Congratulations to both of the winners!**

**GENERAL INFORMATION**

Meals each weekday: Breakfast - 6:45- 8:00  
Lunch - 12:00 noon- 1:30  
Dinner - 5:30 - 6:30 (except Thursday)

Sessions: All morning sessions start at 8 AM. Evening sessions start at 7:00 PM. There will be a break, with refreshments approximately from 9:45-10:15 during each morning session, and no scheduled breaks during the shorter evening sessions.

Sunday - Thursday: After the evening sessions, there will be informal gatherings in Laird Hall, with refreshments provided by sponsors.

Sunday - Thursday: The swimming pool will be available from 1:30-4:30 each day with a lifeguard.

Monday, Tuesday, Thursday: At 3:00 PM each day, a walk/run contest will be organized, beginning at the sundial. Prizes will be awarded at the banquet for those who can estimate their time the closest. Information on a walking tour of historic Chambersburg, which you can try on your own during your free time, will be distributed to all delegates at registration. Golf outings are also planned. The bus trips are on Wednesday afternoon. Sign up in dining hall.

Tuesday: Poster presenters will be with their posters in Laird Hall from 1:30-3:30.

Wednesday: Change of towels and wash cloths. Place dirty linen outside your door.

Thursday: Special vendor workshops in the Science Center, rooms 113,123, and 129.

Thursday: 1:00 - 2:00, Board Room, McElwain Hall - Council for Near Infrared Spectroscopy, planning for IDRC 2000.

Messages: Post on bulletin board in dining hall lobby. For incoming messages, ask callers to dial 717-264-4141 and follow instructions. For Faxes, ask senders to call 717-264-1578.

Photocopies: There will be a code for copies made at the post office in Edgar Hall.

Departures: Sign up for return rides on Friday to the airport of your choice. Sign up sheets for offers and needs will be on the bulletin board near the dining room entrance.

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