

## **Tenth IDRC Conference – 2000**

### **Chairman: Franklin E. “Woody” Barton III**



#### IDRC 2000 Tenth Chambersburg Conference

The tenth IDRC was a big meeting. We literally filled the halls. Dormitory space was filled and downtown motels handled the overflow. The total delegate count was over well 200 and each session was full. I remember two things about this meeting. The first was that we hauled a lot of equipment and stuff from Athens, GA to Chambersburg, PA. In all four large government vehicles were filled with computers, projectors and all the handouts for the meeting. We ran out of notebooks and Foss/NIRSystems had more driven up from Silver Springs so everyone would have a notebook. The second thing I remember is the program spread in NIR News vol.11, No.4 (pages 10-11) showed me with some brown hair. What I remember most is the hard work put in by Sandra Kays, Dave Himmelsbach, Bob Windham, Farris Poole, Judy Davis and Doug Archibald. Bob did the posters (and still does), Dave handled other activities, Farris Poole ran the van to pick up delegates and get them places and Judy took care of anything else that was needed. I cannot say enough about the coordination of all the activities to put together the roster of attendees, mailing list, e-mail lists and all the coordination with Wilson College to make it work smoothly and without Sandra Kays it would not have happened.

I remember our really nice shirts we had made. Twin Cat Designs did a great job and got them to us on time. We also ran short and they made a special run and got them to us before the meeting ended. The tenth IDRC was the era of digital cameras. Almost everyone had one and there were numerous photographs taken which have never seen the light of day. In fact I cannot find the ones I took.

The presentation by John Coates was an excellent beginning for the conference and set the tone. The technical sessions followed the usual format for the most part, but there were some unique sessions. John Shenk chaired a session on calibration transfer techniques, which carried presentations by Jon Goode, Bruker and Steve Lowry, Nicolet/Thermo on techniques for interferometers. Tomas

Isaksson had an excellent chemometrics session and Donald Dahm's theory session was also unique. One of my favorites was the banquet speech by Dave Peterson of NASA. Dave always gives an interesting and entertaining lecture and the visuals are really great. Dave retired a while back leaving a big hole in the remote sensing world. The IDRC has always been a meeting for reflection, no pun intended, and this one was no exception. The ideas presented and the discussions of the week had a profound impact on the direction my research has taken. It is time for another boost.

# 10<sup>TH</sup> INTERNATIONAL DIFFUSE REFLECTANCE CONFERENCE

August 13-18, 2000

## WELCOME TO CHAMBERSBURG

### Friday, August 11

5:00-9:00 PM Registration for those attending Saturday short courses - dining hall entrance.

6:30-7:15 PM Dinner

### Saturday, August 12

#### **PRE-CONFERENCE SHORT COURSES** Warfield Rooms 101 and 102, Havens Science Center

9:00 AM-5:00 PM **Introduction to NIR Spectroscopy and Calibrations** - presented by Tony Davies, Norwich Near Infrared Consultancy and Tom Fearn, University College London.

9:00 AM-5:00 PM **Electronics for Spectroscopists** - presented by W. Fred McClure, North Carolina State University.

8:00-9:00 AM Breakfast in dining hall for short course attendees

9:00 AM Short courses begin

10:30 AM Break

1:00-1:45 PM Lunch in the dining hall for short course attendees

2:00 PM Short courses re-convene

3:30 PM Break

5:00-9:00 PM Registration for those attending Sunday short courses - dining hall entrance.

6:30-7:15 PM Dinner for those attending short courses

Sunday, August 13

**PRE-CONFERENCE SHORT COURSES**  
Warfield Rooms 101 and 102, Havens Science Center

- 9:00 AM-4:00 PM** Intermediate Course - Practical PCA, PLS and Wavelength Selection  
- **presented by Michael Bystrom, Camo.**
- 9:00 AM-4:00 PM** Advanced NIR Technology - Instrumentation Review and Algorithms  
for Standardization/Calibration Transfer - **presented by John Coates, Coates  
Consulting and Tom Fearn, University College London.**
- 8:00-9:00 AM** **Breakfast for short course attendees**  
**9:00 AM** **Short courses begin**  
**10:30 AM** **Break**  
**1:00-1:45 PM** **Lunch for short course attendees**  
**2:00 PM** **Short courses re-convene**
- 3:00-9:00 PM** **CONFERENCE REGISTRATION - dining hall entrance.**  
**5:30-6:30 PM** **Dinner for all registrants**

During the remainder of the conference, daily meal schedules are:

- 6:45-8:00 AM** **Breakfast**  
**12:00-1:00 PM** **Lunch**  
**5:30-6:30 PM** **Dinner**

**7:00 PM**

**CONFERENCE OPENING**  
Havens Science Center,  
Auditorium

Plenary speaker, Dr. John Coates

"A REVIEW OF CURRENT AND NEW TECHNOLOGIES FOR NIR  
SPECTROSCOPY"

**8:30 PM**

**INFORMAL RECEPTION**  
Sponsored by Foss NIRSystems  
Laird Hall

Monday, August 14  
8:00 AM -12:00

## TECHNICAL SESSIONS

ORIGINS OF SIGNALS - PHYSICAL AND CHEMICAL EFFECTS Chair: **Donald**

**Dahm, TechMan Enterprises**

Eliminating chemical interferences with coherent 2D DOVE spectroscopy. **John Wright, University of Wisconsin.**

Anomalies in NIR. **Emil W. Ciurczak, Purdue Pharma LP.**

The unpleasant surprises of physical and chemical effects: Stories and discussion. **Tony Davies, Editor, JNIRS, and others.**

**9:45 AM Break**

Seeing through layers. **Georgi Krivoshiev, Canning Research Institute, Bulgaria.**

Correcting calibrations for physical and chemical effects: Examples and discussion. **Lois Weyer, Hercules Inc., and others.**

Practical limitations imposed by particle size in determination of absorption coefficients. **Kevin Dahm, Rowan University.**

**12:00-1:00 PM**      **Sign-up for all afternoon tours - dining room entrance.**

**2:00-3:00 PM**      **Optional afternoon session**  
A hundred and forty years of diffuse reflectance theory: A brief history of the field and a clear, concise explanation of current theory.  
**Donald Dahm, TechMan Enterprises.**

**4:00-5:00 PM**      **Council on Near Infrared Spectroscopy Meeting (CNIRS). The meeting is open to all participants of the conference.**

**7:00-9:30\* PM**

**MEASUREMENT OF INSTRUMENT PERFORMANCE** Chair: **Bob**

**Windham, USDA-ARS**

Procedures for evaluating spectrometers for noise, bandpass, wavelength accuracy and precision. **Karl Norris, Beltsville, MD.**

Standards and software for NIR hardware validation. **William Muller, Foss NIRSystems.**

NIST artifact calibration standards for the NIR. **Steven Choquette, John Travis, David Duewer, ChangJiang Zhu, National Institute of Standards and Technology.**

Spatial and spectral calibration procedures for hyperspectral imaging spectrometers. **Kurt Lawrence, Bosoon Park, USD A, ARS.**

Verification of spectroscopic performance during the design phase of a new FT-NIR spectrometer. **Steve Lowry, Mark Kemper, Bill McCarthy, Ed Magnuson, Nicolet Instrument Corporation.**

**9:30 PM**                      **INFORMAL RECEPTION** - Sponsored by David Hopkins  
Laird Hall

Tuesday, August 15

**8:00 AM-12:00**

**ORIGINS OF SIGNALS - BIOMEDICAL AND LIFE SCIENCES APPLICATIONS** Chair: **Roumiana**

**Tsenkova, Kobe University**

NIR imaging: An emerging technology for tissues. **Britton Chance, University of Pennsylvania.**

New hybrid multivariate algorithm for NIR spectral analysis of analytes of clinical importance. **David Haaland, Sandia National Laboratories.**

Spatial and depth related information from NIR reflectance measurements of tissue *in vivo*: Key factors in providing clinically relevant information. **Michael Sowa, Institute for Biodiagnostics, National Research Council (Canada).**

**9:45 AM Break**

Evaluation of physiological condition of ruminant animals by NIR spectra of body liquids.

**Steffka Atanassova, Tracia University, Bulgaria.**

Diffuse reflectance spectroscopy in medicine: Clinical applications of near-infrared optical tomography.

**Mamoru Tamura, Hokkaido University.**

Optical topography for higher-order brain function analysis. **Hideaki Koizumi, Hitachi Advanced Research Laboratory.**

Near IR biospectroscopy: A window on metabolism. **David Burns, McGill University.**

**1:30-3:30 PM** POSTER PRESENTATIONS - Laird Hall.

**7:00-9:30 PM**

INSTRUMENT PERFORMANCE - VENDOR EVENING Chairpersons:

**Susan Foulk, Guided Wave and Howard Mark, Mark Electronics Company**

**representatives will give short presentations as part of the program.**

9:30 pm INFORMAL RECEPTION - Sponsored by Bran + Luebbe  
Laird Hall

Wednesday, August 16

**8:00 AM-12:00**

CHEMOMETRICS - QUANTITATIVE AND QUALITATIVE ASPECTS Chair: **Tomas**

**Isaksson, Agricultural University of Norway**

On-line solids composition monitoring by NIR: The journey from theory to practice.

**Charles Miller, John Hawkins, DuPont Central Research; Cleveland Johnson, Larry Bailey, E. Stridde, DuPont Packaging and Industrial Polymers.**

Variable selection in PLS regression by use of jack-knife based significance testing. **Frank Westad, MATFORSK.**

**9:45 AM Break**

When is an SEP really better than another SEP? **Tom Fearn, University College London.**

Discriminant analysis. **Tomas Isaksson, Agricultural University of Norway.**

Strategic selection of samples with great seasonal variation. **Christel Solberg, Bodo College, Norway.**

**Discussion**

**12:15PM-6:30 PM EXCURSIONS**  
Pennsylvania Dutch Country, Lancaster, PA Outlet Mall,  
Hershey, PA  
**See information in the registration packet**

**7:00-9:30 PM**

**CHEMOMETRICS - SOFTWARE SHOOTOUT Chair: Fred**

**McClure, North Carolina State University**

Formal and informal participants will present their results on a data set posted on the web site. Scheduled participants are:

**Howard Mark**  
**Tony Davies**  
**Sumio Kawano**

**9:30 PM** **INFORMAL RECEPTION - Sponsored by Textron Systems**  
**Laird Hall**



Thursday, August 17  
8:00 AM-12:00

## CALIBRATION AND SPECTRAL TRANSFER

Chair: **John Shenk, Infracsoft International, LLC**

Assessing the relative transferability of ANN and PLS calibrations. **Dave Funk, GIPSA.**

Accuracy and transferability comparison of various multivariate processing algorithms for corn quality assessment. **Sylvie A. Roussel, Glen R. Rippke, Charles R. Hurburgh, Jr., Iowa State University.**

Factors that influence direct calibration transfer in NIR analysis. **Jon Goode, Sameer Londhe, Qian Wang, Bruker Optics.**

**9:45 AM Break**

The effect of hardware and software design on calibration transfer in a new FT-NIR spectrometer. **W.J. McCarthy, G.L. Ritter, S.R. Lowry, Nicolet Instrument Corp.**

Calibration transfer experiences. **John Shenk, M.O. Westerhaus, Infracsoft International, LLC. Inc.**

Platform and spectral region issues for calibrations. **F.E. Barton, II, D.S. Himmelsbach, USDA-ARS.**

**7:00-10:00 PM**

## BANQUET

Wines sponsored by NIR Publications

Speaker, David L. Peterson,  
**N.A.S.A., Ames Research Center.**

"PROGRESS IN APPLYING NIRS TECHNIQUES TO REMOTE  
SENSING OF THE EARTH."

Friday, August 18  
**8:00-11:30 AM**

NOVEL APPLICATIONS AND APPROACHES

Chair: **Lois Weyer, Hercules, Inc.**

A hand-held NIR instrument based on gap-second derivative theory. **Susumu Morimoto, Kubota Corp.**

Experiences with a new instrument operated on a combine harvester. **Phil Williams, Canadian Grain Commission.**

Dynamic and automated polarized NIR polymer spectroscopy. **David L. Wetzel, Kansas State University, Manhattan, KS**

**9:45 PM Break**

Near-infrared imaging - one detector, no moving parts. **Bill Fateley, Three LC, Inc.**

A kromoscopic instrument for non-invasive blood glucose measurement. **Howard Guthermann, Optix.**

A novel mathematical approach for NIR non-invasive measurement. **Bob Rosenthal, Futrex.**

**11:30 AM-12:00**

ELECT IDRC 2002 CHAIR Adjourn

## POSTER PRESENTATIONS

### Laird Hall

Authors will be present at posters on Tuesday from 1:30-3:30 PM Posters are also available for viewing in the afternoons and during the evening receptions

**Identification of genetically modified grains by near infrared spectroscopy.** Charles R. Hurburgh, Jr., Connie L. Hardy, Sylvie A. Roussel, Glen R. Rippke, Iowa State University, Agricultural and Biosystems Engineering, Grain Quality Laboratory, 1563, Food Sciences Bldg., Ames, Iowa 50011-1061.

**Near Infrared transreflectance spectroscopy (NIRS) method for a fast determination of polyphenolic compounds.** C. W. Huck and G. K. Bonn. Institute of Analytical Chemistry and Radiochemistry, Leopold-Franzens University, Innrain 52a, 6020-Innsbruck, Austria.

**New method for potato sorting.** Georgi Krivoshiev, Raina Chalucova, Mihail Moukarev, Canning Research Institute. Section Food Quality and Safety, 154 Vassil Aprilov Blvd. Plovdiv 4003, Bulgaria.

**Rapid and simple determination of undesirable constituents (nitrate and soluble oxalic acid content) in spinach by short-wave near infrared spectroscopy.** C. Iyo, K.C. Seong\*, S. Kawano, National Food Research Inst, Tsukuba 305-8642, Japan, \*National Horticultural Research Institute, Suwon 440-310, Korea.

**Analysis of goat's blood by NIR diffuse reflectance spectra measured using a blood collecting tube as a sample cell.** S. Kawano, C. Iyo, F. Terada\*, National Food Research Inst., Tsukuba 305-8642, Japan, \*National Institute of Animal Industry, Inashiki 305-0910, Japan.

**Preliminary study on NIR detection of rice quality deterioration during storage using NIR spectra of brown rice whole grains.** M. Fukami and S. Kawano\*, Tsukuba University, Tsukuba 305-8572, Japan \*National Food Research Inst., Tsukuba 305-8642, Japan.

**Assessing comparative performance and calibration transferability of a NIRS diode array and a NIRS grating instrument (Zeiss Corona NIR 1.7 vs. NIRSystems 6500) on dried forages.** Michael Rode and Pierre Dardenne, Federal Agricultural Research Centre, Institute of Crop and Grassland Science, Bundesalle 50D-38116 Braunschweig, Germany.

**Forage analysis in the field by NIRS diode array instrumentation.** Christian Paul, Michael Rode and Ulf Feuerstein, Federal Agricultural Research Centre, Institute of Crop and Grassland Science, Bundesalle 50 D-38116 Braunschweig, Germany

**Near infrared transmission study for fresh grass silage analysis.** Christian Paul, Manfred Sommer and Uwe von Borstel, Federal Agricultural Research Centre, Institute of Crop and Grassland Science, Bundesalle 50 D-38116 Braunschweig, Germany.

**Application of near-infrared spectroscopy to measurement of moisture, carbon and nitrogen content during compost fermentation.** Ken-ichiro Suehara, Department of Information Machines and Interfaces, Faculty of Information Sciences, Hiroshima City University, 3-4-1, Ohzukahigashi, Asaminami-ku, Hiroshima 731-3194, Japan.

**Jack-knifing for evaluation of wavelengths.** Christel Solberg, BOD0 College, 8049 BOD0, Norway.

**Kromoscopic analysis in print.** M.W. Misner, H. Guthermann and M.J. Block, Optix, LP.

**The development of a tabletop fruit taste meter.** Susumu Morimoto Research & Development Dept. Kubota Corp. 1-1, Hama-Ichome, Amagasaki-shi Hyogo, 661-8567, Japan.

**Mastitis diagnosis by means of NIR cow milk and urine spectra and SIMCA classification.** Stefka Atanassova, Department of Mathematics and Physics, Thracian University Student Town 6000 Stara Zagora, Bulgaria.

**Application of near-infrared spectroscopy to measurement of moisture, carbon and nitrogen content during compost fermentation.** Ken-ichiro Suehara, Department of Information Machines and Interfaces, Faculty of Information Sciences, Hiroshima City University, 3-4-1, Ohzukahigashi, Asaminami-ku, Hiroshima 731-3194, Japan.

**Qualification of food flavours using NIR spectroscopy and chemosensor-array (electronic nose).** Zsolt Seregely, University of Horticulture and Food Industry, H-1118 Budapest, Menesi ut45.

**Qualification of volatile oils using NIR and electronic nose.** Gabriella Kisko, University of Horticulture and Food Industry, H-1118 Budapest, Somloi ut 14-16.

**Monitoring the effect of the "ultra-high pressure" preservation technology by near infrared reflectance spectroscopy.** Karoly J. Kaffka, University of Horticulture and Food Industry, H-1118 Budapest, Menesi ut 45.

**Effect of sample diversity on mid- and near-infrared diffuse reflectance calibrations for carbon in soils.** J.B. Reeves, III, G.W. McCarty, R.F. Follett, J.M. Kimble, V.B. Reeves, USDA-ARS, Beltsville, MD 20705.

**Combinatorics in environmental analysis - a simple solution to a complex problem. H.** Frickel, Merck KgaA, Darmstadt, Germany.

**Analysis of physico-chemical properties in soils by NIRS.** KwanShig Ryu, BokJin Kim, WooChurl Park, RaeKwang Cho, Department of Agricultural Chemistry, Taegu University, Korea.

**Non-destructive determination of quality in compost by NIRS.** SangHyun Seo, WooChurl Park, RaeKwang Cho, Department of Agricultural Chemistry, Kyungpook National University, Taegu, Korea.

**NIRS for non-invasive measuring of internal quality in apple fruit.** MiRyeong Shon, EunOck Kim, Rae Kwang Cho, Department of Agricultural Chemistry, Kyungpook National University, Taegu, Korea.

**Development of robust calibration for determination of apple sweetness using NIRS.** Mi Ryeong Shon, Eun Ock Kim, Rae Kwang Cho, Woo Churl Park, Department of Agricultural Chemistry, Kyungpook National University, Taegu, Korea.

**Rapid analysis of nutrients and metals in biosolids-amended soils using near-infrared spectroscopy.** D.F. Malley, L. Yesmin\*, and M.R. Banerjee\*, PDK Projects, Inc., 365 Wildwood Park, Winnipeg MB R3T OE7, Canada, \*Semiarid Prairie Agricultural Research Centre, Agriculture and Agri-Food Canada, Swift Current SK S9H 3X2, Canada.

**Near-infrared spectroscopy as a tool for the comprehensive analysis of lake sediments.** D.F. Malley and P. Badiou, PDK Projects, Inc., 365 Wildwood Park, Winnipeg MB R3T OE7, Canada.

**Rapid analysis of nutrient and salt concentrations in hog manure by near-infrared spectroscopy.** D.F. Malley, R.G. Eilers\*, E. Rempel\*\*, M. Van Walleggem\*\*\*, and P.D. Martin, PDK Projects, Inc., 365 Wildwood Park, Winnipeg MB R3T OE7, Canada, \*Land Resource Unit, Brandon Research Centre, Agriculture and Agri-Food Canada, University of Manitoba, Winnipeg MB R3T 2N2, Canada, \*\*Ecolagra Inc., Box 664 Niverville MB ROA 1EO, Canada, \*\*\*Innovan Enterprises, Box 377, Oak Bluff MB ROG 1NO, Canada.

**Near-infrared spectroscopy for the rapid determination of nutrients in soil amended with hog manure.** D.F. Malley, L. Yesmin\*, P.D. Martin, and M.R. Banerjee\*, PDK Projects, Inc., 365 Wildwood Park, Winnipeg MB R3T OE7, Canada, \*Semiarid Prairie Agricultural Research Centre, Agriculture and Agri-Food Canada, Swift Current SK S9H 3X2, Canada.

**Monitoring of powder blend homogeneity using near-infrared.** Arwa S. El-Hagrasy, Hannah R. Morris, Philip Lunney, and James K. Drennen, III, Division of Pharmaceutics, Graduate School of Pharmaceutical Sciences, Duquesne University, Pittsburgh, PA 15282.

**Calibration development using near infrared spectroscopy.** Meenakshy Narayan, Hannah R. Morris, Philip Lunney, Rachel E. Hroncich, and James K. Drennen, III, Division of Pharmaceutics, Graduate School of Pharmaceutical Sciences, Duquesne University, Pittsburgh, PA 15282.

## **IDRC 2000 COMMITTEE**

**Chairman** - Franklin E. Barton, II

**Program** - F.E. Barton, II and Committee

**Short Courses** - Doug Archibald

**Registration and Circulars** - Sandra Kays

**Posters** - Bob Windham

**Activities** - Dave Himmelsbach

**Exhibits** - Howard Mark

**Evening Receptions** - Phil Williams

**CNIRS Treasurer** - Susan Foulk

**CNIRS President, Student Awards Committee Chair** - Jim Reeves

**Web Site Construction** - James Griffin

**Assistance with Registration** - Judy Davis, James Hall and Farris Poole

**IDRC 2000 is sponsored by the Committee on Near Infrared Spectroscopy (CNIRS)**

## **EXHIBITORS**

### **Atech, Inc**

Exhibiting for Karl Zeiss Instruments  
45 John Street, New York, NY 10038  
Phone: 212-393-9540  
Fax: 212-393-9539

### **Bran + Luebbe**

1025 Busch Parkway, Buffalo Grove, IL 60089 Phone: 708-520-0700

### **Buchi Analytical**

19 Lukens Drive, Suite 400, New Castle, DE 19720 Phone: 302-652-3000  
Fax: 302-652-8777 e-mail:  
rubinovitz.r@buchi.com

### **Data Specifics**

3901 Wood Duck Drive, Suite E Springfield, IL  
62707 Phone: 217-789-499

**Foss NIRSystems**

12101 Tech Road, Silver Spring, MD 20904

Phone: 800-343-2036

Fax: 301-236-0134

**Galactic Industries Corp.**

395 Main Street, Salem, NH 03079 Phone: 603-898-7600

Fax: 603-898-6228 <http://www.galactic.com>

**Nicolet Instrument Corp.**

9901-H Business Parkway, Lanham, MD 20706

Phone: 800-237-2800

Fax: 301-731-5761

**Perten Instruments**

6444 South 6th St. Road, Springfield, IL 62707

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