

The NIR Spectrum

Newsletter of the Council for Near Infrared Spectroscopy*

Vol. 4 No. 2



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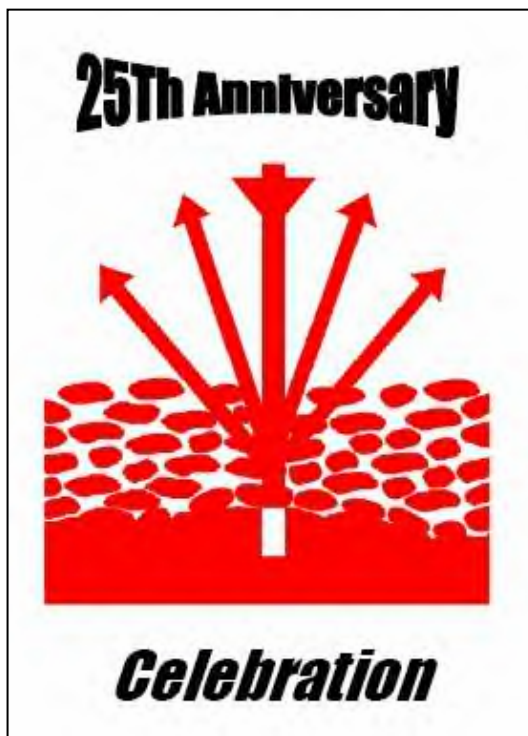
*The Council for Near Infrared Spectroscopy is a Technical Affiliate of the Society of Applied Spectroscopy

The 13th International Diffuse Reflectance Conference (IDRC 2006) Commemorating 25 Years Theory and Design

Dear Conferee,

We welcome each and every one of you to the thirteenth meeting of the International Diffuse Reflectance Conference (13th IDRC 2006) and cordially invite you to attend this years

Chambersburg." The theme this year will be theory and design. The conference is celebrating its twenty-fifth anniversary! You will receive a commemorative book, The 13th International Diffuse



conference. For the price of a movie ticket (ok, a bit of a stretch, but not to far off the mark, right Howie?), you can attend what many have come to believe is "the best kept secret in

Reflectance Conference (IDRC) Commemorating 25 Years of IDRC: Theory and Design, in honor and memory of Gerald S. Birth, the conference founder, recapping the first twelve confer-

ences. Howard and I would like to publicly thank the vendors and private individuals who graciously donated and supported this project, and all the past session chairs and contributing authors who without their support, and their sweat, it would not have been possible. Thank you one and all.

We will kick off the conference on August 5th and 6th with five short courses featuring some of the world's foremost experts within their respective fields. On Saturday, a half day short course on Imaging will be given by Neil Lewis and Linda Kidder, both principals and founders of Spectral Dimensions, Inc. A full day course on Process Analytical Spectroscopy will be taught by Katherine A. Bakeev, of GlaxoSmithKline, and editor of the newly penned text on Process Analytical Technology published by Blackwell Publishing, and Ann M. Brearley, of Brearley Consulting.

On Sunday, a half-day course on Near-Infrared Spectral Interpretation will be taught by Lois Weyer, past chair of IDRC (1998) and recognized for her contributions to IR/NIR spectral interpretation, and Heinz Siessler of the University of Duisburg-Essen, the 2000 Tomas P. Hirschfeld Award recipient, and the 2003 Buechi Award in Near-Infrared spectroscopy. Also, a half-day course will be given on Data Treatment by David Hopkins, who has previously presented training courses on Using NIR Spectroscopy under the auspices of the American Chemical Society and Applied Chemometrics. The first and longest running short course given at Chambersburg, having been given at IDRC since 1996, will be a full day short course on An Introduction to NIR Spectroscopy and Chemometrics,

taught by Tony Davies, of Norwich Near Infrared Consultancy, and Tom Fearn Department of Statistical Science, University College London, UK.

On Sunday at 6:00 PM, the Welcome Reception will be held at the Lenfest Commons to honor and acknowledge our long and very supportive relationship with our host, Wilson College. We will then move to the Science Center Auditorium where Jerry Workman will deliver a keynote address; "Vision, Science Fiction, and Technology in Afterburner: Looking Ahead to the Next 30 Years of Spectroscopy..."

This year's program is diverse, featuring speakers from all over the world, from the far east to the f a r west. In

observed. (The final program accompanies this article.)

A typical day at the conference (see the accompanying schedule) will begin with breakfast served from 7:00 – 8:00 AM. Lectures begin at 8:00 AM every morning with a mid-morning break and a break for lunch from 12:00 - 1:00 PM. This year, we will have afternoons open, however, several lounge areas will be available for afternoon discussions (McElwayne, 2nd & 3rd lounges in Davison, the private dining room, and the Patterson Room lounge - all offering a cool haven). Mid-afternoon breaks will take place at the Lenfest Commons lounge and the Patterson Room lounge. The swimming pool will be open in the afternoons Monday through Thursday, from 2:30 - 5:30 PM. The ever popular predict your own time (PYOT) will be run by Fred McClure. The CNIRS will meet at 4:00 pm on Monday, August 7, 2006 in the Patterson Board Room. All are welcome to attend the "Council" meeting.

Dinner will be served from 5:30 - 6:30 PM on Saturday, Monday and Wednesday. Sunday dinner will be served at 5:00 PM to accommodate the Welcoming Reception at 6:00 PM to be held in Lenfest Commons. The much anticipated official poster session will take place Tuesday afternoon after lunch in Laird Hall from 1:00 - 4:00 PM. Participants are encouraged to view the posters each evening during the social hours. A picnic will be held on Tuesday, and the banquet on Thursday, with the Banquet Reception beginning at 6 PM. All evening lectures will begin 7:00 PM and last until we convene in Laird Hall for socializing.

Wednesday evening has been set aside to honor Professor Yukihiro Ozaki, recipient of the Gerald



***The Council for Near Infrared Spectroscopy
Congratulates the IDRC on the Occasion of its
25th Year***

trying to further elucidate the nature of diffuse reflectance phenomenon and perhaps get closer to solving the inverse closed solution form for diffuse reflectance, the speakers will look at the problem from the aspect of the experimental evidence, and the fundamental chemical, physical and mathematical issues that confront the analyst in trying to deduce the absorption and scatter patterns

S. Birth Award. This award is sponsored by Unity Scientific, and is given for Ozaki's outstanding work in advancing the Art and Science of Near Infrared Spectroscopy. The Council for Near Infrared Spectroscopy (CNIRS) is recognizing Professor Yukihiro Ozaki of the Department of Chemistry of Kwansai Gakuin University, Sanda, Japan for the work of his research group in many different aspects of chemometrics. Their work is exemplified by two papers: (1) *Improvement of the Partial Least Squares Model Performance for Oral Glucose Intake: Experiments by Inside Mean centering and Inside Multiplicative Signal Correlation*, Y. Du, S. Kasemsumran, K. Maruo, T. Nakagawa, and Y. Ozaki, *Analytical Sciences*, 21, 979-984 (2005) and (2) *Removal of Interference Signals Due to Water from in vivo Near-infrared (NIR) Spectra of Blood Glucose by Region Orthogonal Signal Correlation (ROSC)*, by Y. P. Du, Y. Z. Liang, S. Kasemsumran, K. Maruo, and Y. Ozaki, *Analytical Sciences*, 20, 1339-1345, (2004).

On Thursday morning, the ever popular shootout session will convene in the Science Center Auditorium. This is an event not to be missed. This year, Fred McClure features the return of Marc Meurens (Lucky Luke - Faster on the draw than his own shadow.) The data set this year was from David J. Brown, Department of Landscape Pedology, Montana State University. Some say it is a data set that only Jim Reeves (Dr. Dirt) could love, there are over 3000 spectra in all, typical of datasets encountered in Pedometrics. There are 2,761 spectra in the calibration/prediction (CAL) set; 1423 spectra in the validation (VAL) set. The spectra come from soil samples collected from all over the USA.

We are in for a treat as we celebrate, reminisce and have a great time at the banquet Thursday evening. This year's speaker, Dr. Warren Vidrine, will instruct, amuse and entertain as we get to peer inside the mind of one of spectroscopy's most colorful fellows. On Friday, I will host presentations on special topics of interest, ranging from NIR analysis of sugarcane in the fields of India



Gary E. Ritchie, IDRC 2006 Chairman

to core samples from the trees of Georgia, USA, and the analysis of some funny money from the pockets of the underground.

We have arranged for transportation to and from Hershey Park and associated sites and Art Springsteen will arrange for conference golfers to have outings throughout the week (also on Wednesday). The field trip details are posted on the website and are as follows: Buses to be ready for departure at 11:45 AM on Wednesday, actual departure at noon. Box lunches will be made available to eat on the buses. The

buses will arrive in Hershey at about 1 PM. They will stop at four locations: park entrance/visitor center/museum botanical gardens outlet shopping area zoo. The buses will circulate once per hour in case anyone wants to visit more than one location. People who get off the bus at the first stop can go to the visitor center, the museum, or the park as they are all within walking distance. Final departure is at 4 PM for return in time for dinner (5:30 pm). The visitor center and outlet shopping are free. The gardens cost \$7 adult/\$4 child. The zoo costs \$8 adult/\$7 child.

The museum is \$7 adult/\$3 child. The park was \$39.95 last year, but IDRC can probably get \$6 off coupons for each person. Youth (ages 3-8) park fees are \$22.95 (minus a \$2 coupon if available). More information on the locations can be seen at:

www.hersheypa.com

David Semmes has graciously volunteered to coordinate rideshares and travel to and from C'burg and the airports. David may be contacted by email at:

dsemmes@gmail.com

We look forward to your stay. If you have any questions, contact me, Gary Ritchie, by phone (301-816-8353), or email:

ger@usp.org

I will also be available onsite for the registration and throughout the conference.

- Gary Ritchie
USP Pharmacopeia
Rockville, MD



IDRC 2006 SCHEDULE

F r i d a y Aug 4	S a t u r d a y Aug 5	S u n d a y Aug 6	M o n d a y Aug 7	T u e s d a y Aug 8	W e d n e s - d a y Aug 9	T h u r s d a y Aug 10	F r i d a y Aug 11
2:00 PM – 5:30 PM Short course Registration (Lenfest Lobby)	7:00 AM - 8:00 AM Breakfast (Cafeteria)	7:00 AM - 8:00 AM Breakfast (Cafeteria)	7:00 AM - 8:00 AM Breakfast (Cafeteria)	7:00 AM - 8:00 AM Breakfast (Cafeteria)	7:00 AM - 8:00 AM Breakfast (Cafeteria)	7:00 AM - 8:00 AM Breakfast (Cafeteria)	7:00 AM - 8:00 AM Breakfast (Cafeteria)
	8:30 AM – 4:45 PM PAT Katherine Bakeev & Ann Brearley (SC 107)	8:00 AM – 4:00 PM Chemometrics Tony Davies & Tom Fearn (SC 107)	8:00 AM - 12:00 PM Experimental Evidence for Diffuse Reflectance: Robert Lodder (SC Auditorium)	8:00 AM - 12:00 PM Chemistry of Diffuse Reflectance: Phil Williams & Charles Hurburgh (SC Auditorium)	8:00 AM - 12:00 PM Mathematics of Diffuse Reflectance: Tony Davies & Tom Fearn (SC Auditorium)	8:00 AM - 12:00 PM Shootout Fred McClure (SC Auditorium)	8:00 AM – 12:00 PM Special Topics: Gary Ritchie (SC Auditorium)
	9:45 AM – 10:15 AM Mid-Morning Break (SC Lobby)	8:00 AM – 12:00 PM Data Handling Dave Hopkins (SC 113)	9:45 AM – 10:15 AM Mid-Morning Break (SC Lobby)	9:45 AM – 10:15 AM Mid-Morning Break (SC Lobby)	9:45 AM – 10:15 AM Mid-Morning Break (SC Lobby)	9:45 AM – 10:15 AM Mid-Morning Break (SC Lobby)	9:45 AM – 10:15 AM Mid-Morning Break (SC Lobby)
	12:00 PM - 1:00 PM Lunch (Cafeteria)	9:45 AM – 10:15 AM Mid-Morning Break (SC Lobby)	12:00 PM – 1:00 PM Lunch (Cafeteria)	12:00 PM – 1:00 PM Lunch (Cafeteria)	11:30 AM – 5:00 PM Hershey Park / Golf	12:00 PM – 1:00 PM Lunch (Cafeteria)	12:00 PM – 1:00 PM Lunch (Cafeteria)
	1:00 PM – 4:00 PM Imaging Neil Lewis & Linda Kidder (SC 113)	12:00 PM – 1:00 PM Lunch (Cafeteria)	2:30 PM – 5:30 PM Open Swim	1:00 PM – 4:00 PM Poster Session Dave Ryan (Laird)	2:30 PM – 5:30 PM Open Swim	2:30 PM – 5:30 PM Open Swim	1:00 PM – 2:00 PM Check out (Lenfest Lobby)
	2:45 PM – 3:15 PM Mid-Afternoon Break (SC Lobby)	12:00 PM – 5:30 PM Conference Check In / Registration (Lenfest Lobby)	2:45 PM – 3:15 PM Mid-Afternoon Break (Lenfest Lobby & Patterson Lounge)	2:45 PM – 3:15 PM Mid-Afternoon Break (Lenfest Lobby & Patterson Lounge)	2:45 PM – 3:15 PM Mid-Afternoon Break (Lenfest Lobby & Patterson Lounge)	2:45 PM – 3:15 PM Mid-Afternoon Break (Lenfest Lobby & Patterson Lounge)	
	5:30 PM – 6:30 PM Dinner (Cafeteria)	1:00 PM – 4:00 PM NIR Interpretation Lois Weyer & Heinz Siesler (SC 113)	4:00 PM - 5:30 PM CNIRS Meeting (Patterson Board Room)	2:30 PM – 5:30 PM Open Swim	5:30 PM – 6:30 PM Dinner (Cafeteria)	6:00 PM – 7:00 PM Banquet Reception (Lenfest Lobby)	
		2:45 PM – 3:15 PM Mid-Afternoon Break (SC Lobby)	5:30 PM – 6:30 PM Dinner (Cafeteria)	5:30 PM – 6:30 PM CNIRS/IDRC Picnic (Lenfest Commons)	7:00 PM – 9:00 PM Birth Award Dave Hopkins (SC Auditorium)	7:00 PM – 9:00 PM Banquet / Speaker (Cafeteria)	

IDRC 2006 SCHEDULE (Cont.)

		4:30 PM – 5:30 PM Dinner (Cafeteria)	7:00 PM – 9:00 PM Physics of Diffuse Re- flectance: Jim Reeves & Don Dahm (SC Auditorium)	7:00 PM – 9:00 PM Exhibitors Evening (Howard Mark (SC Audito- rium)	9:00 PM Social (Laird)	9:00 PM Social (Laird)	
		6:00 PM - 7:00 PM Reception (Lenfest Commons)	9:00 PM Social (Laird)	9:00 PM Social (Laird)			
		7:00 PM – 9:00 PM Conference Opening / Keynote (SC Audito- rium)					
		9:00 PM Social (Laird)					

FINAL SESSION DETAILS

Experimental Evidence for Diffuse Reflectance: Robert A. Lodder

Experimental Observations of Diffuse Reflectance
Robert A. Lodder, Advanced Science and Technology Center, University of Kentucky

DIAL Light Scattering Instrument Systems
Coorg Prasad, Science & Engineering Services, Columbia, MD

Microspectrometric Imaging of Atherosclerosis in Mice and Men
David L. Wetzal, Department of Grain Science and Industry, Kansas State University

Light Propagation in Tissues
Arnold D. Kim, School of Natural Sciences, University of California-Merced

Development of fLCI (Low Coherence Interferometry) as a Clinical Tool for Detecting Malignancy
Adam Wax, Department of Biomedical Engineering, Duke University

Chemistry of Diffuse Reflectance: Phil Williams & Charles Hurburgh

Environment Matters!: Secondary Effects in NIR Spectroscopy
Charles E. Miller, Eigenvector Research Inc., Wenatchee, WA

Near Infrared Spectral Interpretation
Lois Weyer, ATK Elkton, MD

A Chronicle of Assignments for Overtone and Combination Bands of Important Absorbers
Bin Dai, University of Kentucky

Why Non-linearities?
Igor Kovalenko, Iowa State

Spectroscopic Analysis of Matrices
Clay Harris, University of Kentucky

NIRS for biology: Extended Water Mirror Approach
Roumiana Tsenkova, Associate Professor, Kobe University, Japan

Physics of Diffuse Reflectance: Jim Reeves & Don Dahm

Effective Pathlengths of Mid-Infrared Photons through Non-Absorbing and Absorbing Powders
Peter Griffiths & Lacey Averett, University of Idaho

Time-resolved spectroscopy and GASMAS:
Two novel spectroscopic techniques for analysis of highly scattering media
Christoffer Abrahamsson, Lund Institute of Technology

Title to be determined
Dave Burns, Associate Professor, McGill University, Canada

Light Scattering --- Friend or Foe?
Scott Pahl, Senior Scientist, Oregon Medical Laser Center, Univ. of Oregon
Scatter Correction for NIR Diffuse-Reflection Spectroscopy of Solid Materials
Heinz W. Siesler Department of Physical Chemistry, University of Essen

Gerald S. Birth Award Symposium Honoring Professor Yukihiro Ozaki: David Hopkins

Development of New Chemometrics Algorithms for Non-invasive NIR DR Measurement of Blood Glucose
Professor Yukihiro Ozaki, Dean, Kwansai Gakuin University, Sanda, Japan

Mathematics of Diffuse Reflectance: Tony Davies & Tom Fearn

Chemometrics for Novel Spectroscopic Techniques (TRS, SRS):
Applying Chemometrics to Time-Resolved and Spatially-Resolved Spectroscopy
Sylvie Roussel, Ondalys, Montpellier, France

Comparison of Linear and Non-linear Regression Methods in a Complex Agro-food Matrix (Intact Compound Feed)
and a Complex Parameter (Ingredient Percentage): PLS, LOCAL and ANNs Applied to a Large Database
(by video)
Ana Garrido-Varo, University of Cordoba, Cordoba, Spain

CARNAC Applied to the Cordoba Data: An Alternative to Regression Analysis
Tony Davies, Norwich Near Infrared Consultancy, Norwich, UK

An Introduction to Support Vector Machines (SVM): A Discussion of Some (Im)possibilities and Practical
Considerations of SVMs
Uwe Thissen, TNO, The Netherlands

Discriminate Analysis and Quantification Using SVM
Pierre Dardenne, CRA-W, Gembloux, Belgium

SVM Applied to the Cordoba Data
Tom Fearn, Department of Statistical Science, University College London, London, UK



Special Topics: Gary E. Ritchie

Direct determination of sugar in sugarcane using near infrared diffuse reflectance spectroscopy
Ranjana Mehrotra, Scientist, National physical Laboratory, New Delhi, India

Counterfeiters: Catch 'em with Near-IR.

Don Burns, Staff Scientist at Los Alamos National Laboratory, Los Alamos, NM

Application of Lambert's Law in NIR Diffuse Reflectance Spectroscopy
Marc Meurens, University of Louvain, UCL/AGRO/BNUT- Spectrolab,
Croix du Sud 2 (8), B1348 Louvain-la-Neuve, Belgium

High resolution scanning of radial strips cut from increment cores by near infrared spectroscopy
L. R. Schimleck, Warnell School of Forestry and Natural Resources
The University of Georgia, Athens, GA

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SHORT COURSES

(See the IDRC Website - <http://www.idrc-chambersburg.org> - for Details)

An Introduction to NIR Spectroscopy and Chemometrics

(Full Day, Sunday)

Tony Davies Norwich Near Infrared Consultancy, 75 Intwood Road, Cringleford, Norwich NR4 6AA, UK
Tom Fearn Department of Statistical Science, University College, London, UK

Data Treatment

David W. Hopkins, NIR Consultant

Imaging

E. Neil Lewis, Spectral Dimensions, Inc., Olney, MD

Linda Kidder, Spectral Dimensions, Inc., Olney, MD

Near-Infrared Spectral Interpretation

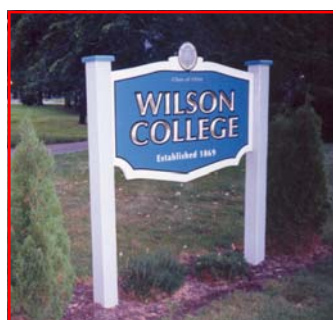
Heinz Siesler, University of Duisburg-Essen, Germany

Lois Weyer, ATK Tactical Systems, Elkton, MD.

Process Analytical Spectroscopy

Katherine A. Bakeev, GlaxoSmithKline, King of Prussia, PA

Ann M. Brearley, Brearley Consulting, Plymouth, MN



**Venue
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