Fourth IDRC Conference – 1988
Chairman: W. F. McClure

The International Diffuse Reflectance Conference:
From Beginnings to New Beginnings

by

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BEGINNING

The first meeting of the International Diffuse Reflectance Conference (IDRC or "The Chambersburg Meeting") was held in August, 1982. However, planning for this meeting started two years earlier – in the mind of Dr. Gerald S. Birth, a researcher with the USDA, Russell Research Center, Athens, Georgia. Gerry was interested in NIR instrumentation and NIR applications but he had a passion for *scattering theory* – a problem that cuts across all molecular spectroscopies. He wrote two of the best references I have ever seen dealing with the interaction of electromagnetic energy with matter.[1; 2] These two paper are classics today.

In 1980 I was invited to Athens to participate in a workshop on near-infrared spectroscopy (NIRS). It was a small group and was held in a conference room on the 7th floor of the Russell Research Center, fondly referred to as "the Russell Hilton." At the end of that meeting, Gerry unloaded his vision of an International Diffuse Reflectance Conference (IDRC) that would convene people who wanted to study "light scattering." Even then, Gerry knew that the key to robust calibrations, ones stand the test of time, was limited by an immature theory of energy scattering. Only two books had been written, one by Wendlandt & Hecht[3] and another by Kubelka-Munk.[4] Birth had both copies and he often complained of their limitations.

No one at that meeting applauded Gerry's vision. We did not disagree but we did not agree. We came away leaving the matter in his hands, knowing full well that if it was to be done, Gerry would have to do it.

PATTERN

I was in my lab in 1981 when I received a call from Gerry. He had driven to Washington, DC to meet with the Board of Directors of the Gordon Research Conferences (GRC). The GRC, a nonprofit organization managed by members of the scientific community, provides an international forum for the presentation and discussion of frontier research in the biological, chemical, and physical sciences, and their related technologies. They hold plenary meetings in the morning and in the evening with the afternoons devoted to small-group technical interchange or recreation. It is a pattern borrowed for the IDRC, the pattern that the IDRC follows today.

Gerry asked the GRC to take the IDRC *under its wing* as an official GRC member meeting. The GRC denied his request stating that "diffuse-reflectance (DR) was too specialized and probably would not maintain a sufficient following to survive scientific scrutiny."

Birth was not deterred by this negative response. He moved quickly with plans to convene the first IDRC in 1982. Few of us volunteered to help Gerry at that time, thinking that it would be difficult to get enough people to hold a conference. Still, Gerry pushed ahead with his plans. My failure to volunteer, much to my disappointment, resulted in being blacklisted for the formal program at the IDRC-1982. Simply stated, I was not invited to present my work.

VENUE

Gerry made a detailed study of the location of people working in the area of optical properties of energy-scattering materials, determining that the population center for those confronted with diffuse reflectance problems lay within a radius which had as its center Chambersburg, Pennsylvania. Guided by a GRC policy of using the facilities of small private colleges, Gerry quickly closed in on Wilson College, a small girls-school on the north side of Chambersburg. On his own recognizance, Gerry immediately booked Wilson College for the first IDRC to be held in August, 1982.

OBJECTIVE

In Gerry's mind, the IDRC was to be the brain trust for all spectroscopies confronted with "energy-scattering problems." It was to include NIRS but it <u>was not</u> to be dominated by NIRS. All sessions were to emphasize scattering problems. As it turns out, the problems faced in NIRS and resulting solutions have spill over into other spectroscopies. For example, mathematical pretreatment of spectral data as well as the use of multivariate statistics for calibration was an <u>NIR first</u>. Data compression methods were first applied to NIR spectra. Modern concepts of data mining were

explored first by NIR spectroscopists. Today these techniques are used in FTIR, Raman and other spectroscopies. Nonetheless, you heard it first in near-infrared spectroscopy.

MARRIAGE

In the summer of 1990, the Council for Near Infrared Spectroscopy and the International Diffuse Reflectance Spectroscopy were made one, with the CNIRS taking responsibility for the management of the IDRC. This *marriage* was announced in the October, 1990 issue of *NIR news*:

CNIRS to sponsor "Chambersburg"

An agreement has been made between the Council for Near Infrared Spectroscopy (CNIRS) and the trustees (previous conveners) of the International Diffuse Reflectance Conference (IDRC, normally known after the town in Pennsylvania, USA where it is held – Chambersburg).

This provides a financial safeguard for future Chambersburg conferences. Until now, the five Chambersburg conferences have been organized on an *ad hoc* basis which meant that the conveners could have been liable for any financial loss.

With this sponsorship agreement, the convener of the 1992 IDRC, Bob Taylor, will be able to sleep more easily!

NIR news 1(1): 22

This has been an amicable relationship that is now going into its 16th year. CNIRS has provided the framework where management issues, business and communications transpire. The IDRC brought to the CNIRS the much-needed venue for training (short courses, etc), technological exchange (posters, session, exhibits and personal networking, etc.) for a broadband of expertise. The two entities alone would never be as strong as the combination. Indeed, it has been a happy marriage.

MILESTONES

Having served at different times, both as President of the CNIRS and Chair of the IDRC, I am convinced that both organizations are very special. CNIRS has not grown tremendously in numbers (ranging for twenty to more than 150 members), but there has always been a faithful few who had visions of a strong and viable organization and have worked to make it great. Several activities have proven to be a unique

contribution of CNIRS/IDRC, benefiting the scientific community. A few are listed here:

Bibliography. David Honigs established the CNIRS Bibliography (CNIRS-B). When Fred McClure took over this database, it included 356 citations. The CNIR-B has always been a money maker for the CNIRS. At last count, more than 67 copies have been delivered, not one has had to be recalled and there has not been one complaint. Today, there are more than 32,000 citations related to NIR technology, chemometrics and other related subjects, covering the time span from 1800 to present day.

Fourier Transform. Between the 1979 and the spring of 1982, my colleagues and I at NC State University had formulated the advantages of Fourier analysis of NIR data. Of the 15 or so advantages, the one that was most impressive at that time was that we could get good agricultural calibrations from the first eleven Fourier coefficients from a Fourier transformation of the NIR spectra in a data set. This represented a data compression ratio of 98%, comparing the data in the wavelength domain vs. data in the Fourier domain.[510]

In July before the first IDRC in August, I went to Gerry begging him to allow me to present my work at the IDRC. Not wanting to see a grown man cry, Gerry agreed to allow me thirty minutes during an evening session. At the conclusion of my presentation you could have heard a pen drop. You see, at that time computers were memory limited. Calibrations could not be easily generated for large data sets. However, with a 98% reduction in storage requirements – this was a significant impact. The thing I recall, that was quite flattering, was that Peter Griffiths was surprised by the results. Yet, later he supported our publication of the findings.[5; 6] Tomas Hirschfeld was complimentary.[11]

Web Page. Bruce Campbell began talking about a “bulletin board” in the early years ago of CNIRS. Bulletin boards were unwieldy and unfriendly to users. Hence, a workable model never materialized. Bruce, a CNIRS members, began hosting small-group discussions (this group soon became referred to as the “Camp Clan,” honoring its founder) at EAS and PITTCON, which provided a venue for discussing of problems encountered in the NIR field. About this same time, Ian Michaels and Tony Davies (NIR Publications, UK) approached Bruce with a proposal to sponsor a Clan forum on a server based in England. Bruce agreed to this arrangement and further discussions of bulletin boards were dropped.

Recognizing that the CNIRS/IDRC could not conduct business on the Camp-Clan Forum, the CNIRS continued to look at options for a Council Website. In 1993, Rob Lodder agreed to host the first official CNIRS web page, on a computer purchase by CNIRS, at the University of Kentucky. Though this site is inactive it is still may be opened with the following URL:

http://www.pharm.uky.edu/asrg/cnirs/hopkins.htm

The last entries were made in 1997, announcing that Jim Reeves was President-Elect of the CNIRS and announcing the next meeting of the CNIRS to be held at the next PITTCON. With no activity, a link to the current website (Susan Foulk, Web Master) was added as follows:

http://www.idrc-chambersburg.org/

Susan Foulk established the current website which, under her guidance, continues to undergo revision and upgrading. With her dedication and support, the CNIRS website is now a viable instrument for conducting Council business, providing technical information to CNIRS members and sharing the "good news" of NIR spectroscopy around the world.

Newsletter. Beginning in 1986 under the name, North American Overtones, the newsletter for the CNIRS soon became an indispensable part of a framework that held the CNIRS and the IDRC together. Not only did it provide a link between the Board of Governors and the membership, it was also a link to other societies. Copies of the NAO were always distributed at PITTCON and EAS. However, as the CNIRS grew in number, interest in a viable newsletter fell – leaving the CNIRS without a regular newsletter from 1991 to 2003. During this same time interest in the CNIRS tapered off to about 20 paying members in the winter of 2003.

Returning from the 11th International Conference for Near Infrared Spectroscopy, held in Cordoba, Spain in 2003, Fred McClure volunteered to accept the Chair of the Membership Committee. During a brief discussion with Woody Barton, it was determined that there were two basic reasons for the lack of interest in the CNIRS: (1) Previous members felt they were getting nothing for their membership money and (2) Members and potential members did not know what was happening within the CNIRS. It was clearly apparent that re-establishing a newsletter would provide a much-needed instrument for recruiting new members as well as keeping current members abreast of what is happening in NIR spectroscopy and diffuse-reflectance worlds.

In 2003, the CNIRS newsletter was revised under the name "*The NIR SPECTRUM,"* a name proposed by Howard Mark and selected by vote of the CNIRS membership. The year 2006 constitutes the 4th year for this quarterly publication. In 2005, per request of NIR Publications, the CNIRS agreed make *The NIR SPECTRUM* a "member-only medium." Issues starting with Vol 3 No 1 require a password in order to access. All issues are stored on the CNIRS/IDRC website at:

http://www.idrc-chambersburg.org/

MOST for the MONEY

Nowhere can you find a scientific conference where you get so much for so little. From the beginning, the cost benefits ratio of the IDRC has been low. It still is. For

example, registration for IDRC-2006 is only $500 for a five-days conference – and that includes everything – room, meals, technical sessions, exhibits and socials – plus access to recreation facilities on one of the most beautiful campuses in the northeast USA.

Convening for a full five days, the IDRC has always followed the Gordon-Conference format – holding plenary sessions in the morning and evening with the afternoon off for one-on-one exchanges and/or recreation. After each evening technical plenary session, attendees gather socially around the exhibits and posters for fun, fellowship and the furtherance of the technology – a time to get to know the people involved in fascinating field.

I have not missed an IDRC. Technical sessions and one-on-one discussions have always generated more ideas that I could pursue during the two years between conferences. There have been occasions when I would hasten home to try new ideas, all stimulated by what transpired at the IDRC. I have been blessed with new friends who have helped me far more than I have helped them. It is my conviction that the CNIRS/IDRC is more than a technical society or an event – it is a technical family – filled with people ready to give of themselves to make sure you too enjoy diffuse reflectance and especially near-infrared spectroscopy.

NEW BEGINNINGS

We stand now inside the threshold of a new century. Not only is there talk, there is also ample evidence that CNIRS/IDRC will have to adapt to new changes, changes that will allow the CNIRS and the IDRC to be more effective than it has in the past.

One of the changes being considered is the shift from printed media to web media. Printed journals and newsletters are struggling to survive. Efforts to stay in business involve shifting from printed copy to electronic copy. Once difficult to produce, training material can be developed on a personal computer and transferred to a website for all to see. Newsletters are a dime a dozen and only those that effective use of the web will survive. However, just the shift to the web will not do the job. New generation websites will have to provide information in an attractive, compact and effective format – arranged in a way and supported with tools that allow the reader to get an overview while at the same time sifting out specific thing of interest. The new reader will not submit to the burden of having to wade through a complete book, paper or article – readers of the future will demand *time-efficient media*. This is why *The NIR SPECTRUM* has been so well accepted. It makes use of the web for distribution, it is indexed and it is techno-personal – that is, readers not only benefits from accessible technical information but they also get to know the authors.

CNIRS may have to change it name. In 2003, the International Conference on Near Infrared Spectroscopy (ICNIRS) changed its name to International Council on Near Infrared Spectroscopy (still ICNIRS) at their meeting in Cordoba, Spain. Now, without doing anything, the CNIRS appear (at least in name) to be a subset of the International CNIRS, now a recognized international body. It is time to consider a

name change that would take the CNIRS to a new level and out from under the umbrella of ICNIRS where it can shine in it own light.

CNIRS is looking to develop its role as an affiliate of other societies. There are advantages to becoming an affiliate, but those advantages must be weighed against the impact they will have on the CNIRS image. Do not forget, CNIRS is where it is today – an established and viable organization with an exciting membership standing on a sound financial footing – because of the hard work and commitment of it members. It is today a highly respected professional organization in and of itself. Relationships with other professional groups will be good as long as there are mutual benefits.

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4TH INTERNATIONAL CONFERENCE ON DIFFUSE REFLECTANCE SPECTROSCOPY AUGUST 14-19, 1988

WELCOME

to the

4th INTERNATIONAL CONFERENCE ON DIFFUSE REFLECTANCE
WILSON COLLEGE
CHAMBERSBURG, PENNSYLVANIA, USA
August 14-19, 1988

We trust that our meeting together like this will be of benefit to you and that your stay here will be a pleasant one. If there is anything we can do to enhance your participation in this conference, please do not hesitate to contact any of us.

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4th INTERNATIONAL DIFFUSE REFLECTANCE CONFERENCE
WILSON COLLEGE
CHAMBERSBURG, PENNSYLVANIA, USA
August 14-19, 1988

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TO EXHIBITORS:

We would like to extend to each and every one who participated in the exhibits our deep appreciation for your support of the 4th International Diffuse Reflectance Conference held at Wilson College, Chambersburg, PA August 14-19, 1988.

The extra income generated from your exhibits has made it possible for us to: 1) invite more international speakers 2) provide reduced conference registration for students doing research in spectroscopy. The conference has become a true international event.

Thank you one and all for your time and exhibits.

THE CONFERENCE COMMITTEE

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NEWSLETTER # 1

4th INTERNATIONAL CONFERENCE ON DIFFUSE REFLECTANCE
WILSON COLLEGE
CHAMBERSBURG, PENNSYLVANIA, USA August 14-19, 1988

PLANNING MEETING

A planning meeting for the 5th International Diffuse Reflectance Conference will be held in the auditorium of the Science Center on Wednesday, August 17, 1:00 PM. Members of the conference who wish to take part in this meeting should be present.

AFTERNOON DISCUSSIONS

A good place to hold your afternoon small group meetings is in the lobby of Prentis Hall. You are encouraged to use this facility from 1-3:00 PM.

MUSEUM

The Museum will be open Tuesday, August 16 from 1:30-3:30 PM for your viewing pleasure.

PHYSICAL FITNESS

Walk/Jog/Run - In 1986 we held the first walk/jog/run event in conjunction with this conference. Tony Davies took the IDRC Walk/Jog/Run Cup; Tony is back again this year to defend his title. Remember, the event is set up for walkers, joggers and runners to compete because the winner is the one who predicts his time required to go the 3 mile course. Monday, Tuesday and Wednesday you will be able to calibrate "your system"; Thursday we will hold the competition. Prizes will be awarded at the banquet. See Fred McClure on center field in front of the dining hall Monday afternoon, August 15 at 4 PM if you plan to participate.

GOLF

Bob Taylor will coordinate the golf again this year. Would you believe he has already checked out all the courses in the area. Meet with Bob Taylor after lunch in the lobby of the dining hall on Monday (1PM), August 15.

VOLLEY BALL

Peter Griffith comes all the way from California to arrange the volleyball tournament this year. So, meet with Peter on center field at 3 PM, Monday, August 15 to choose teams.

TENNIS

Mark Ohura comes from Japan to arrange our tennis match this season. I hear he's a pretty tough on the court. Tennis players schedule your court times with him.

Have a good week. If we can help you, let us know.

SWIMMING

There is no competition swimming planned. The pool, located in the basement of the dinning hall, will be open from 2-5 PM each afternoon except Friday, August 19.

4th INTERNATIONAL
DIFFUSE REFLECTANCE
CONFERENCE

August 14-19, 1988

CONFERENCE PROGRAM

THEME

Diffuse Reflectance Spectroscopy: Analyses in Situ

WILSON **COLLEGE**
CHAMBERSBURG, PENNSYLVANIA, USA

August 14 - SUNDAY EVENING

INAUGURAL SESSION (7 PM): Diffuse Reflectance Spectroscopy

Chairperson: David Wetzel, Dept. of Chemistry
Kansas State University, Manhattan

Peter R. Griffiths, Univ. of Calif., Riverside, CA
"Diffuse Reflectance in the Mid Infrared" *David Honigs, Univ. of Wash., Seattle, WA*
"The Use of Single Fiber Optics for Diffuse Reflectance Measurements" *Franklin E. Barton, USDA/ARS, Athens, GA*
"The Future of Agricultural Analysis" *Howard Mark, Bran+Lubbe, Elmsford, NY*
"XRF for Routine Analysis"

D. L. Wetzel, Kansas State University, Manhattan
"Quantitative Molecular Microspectrofluorimeter in Heterogeneous Solids"

August 15 - MONDAY MORNING

SESSION 2 (8 AM): Interaction of Light and Matter

Chairperson: Gerald Birth, USDA/ARS, Athens, Georgia

Richard G. Leffler, USDA/ARS, Athens, GA
"Diffuse Reflectance: A Qualitative Picture" *Wilford N. Hansen, Utah State University, Logan, UT*
"Pure Physics and Applied Spectroscopy: A Useful Combination" *Gerald Birth, USDA/ARS, Athens, GA*
"Light Scattering in Diffusely Reflecting Materials" *Timo Hyvarinen, Tech. Res. Centr., Oulu, Finland*
"Modeling Diffuse Reflectance by Delta-Eddington Approximation"

August 15 - MONDAY EVENING

SESSION 3 (7 PM): On-Line Spectroscopy

Chairperson: Lois Weyer, Hercules Research Center Wilmington, DE

James B Callis, Univ. of Wash., Seattle, Washington
"Fifth Era in Process Analytical Chemistry"
John S. Huizinga, 3M Co., St. Paul, MN
"Application of Infrared and Near Infrared Spectroscopy to the Online Monitoring of Thin Coatings"
E. *A. Hosegood, Dupont Company*
"Capabilities and Reliabilities of Diffuse Reflectance NIR Spectroscopy to Online Measurements" *Donald A. Burns, Consulting Chemist*
"Liquid Analysis via NIR: Near-line, At-line, On-line or In-line"

August 16 - TUESDAY MORNING

SESSION 4 (8 AM): *New Software in Diffuse Reflectance Spectroscopy*

Chairperson: Mr. A. M. C. Davies, Oxford Analytical Instruments Ltd., Oxon, England

Mark Westerhaus, Infrasoft Int., College Park, PA
"New Software from Infrasoft" Brian Davies, Glaxo Opns. Ltd., United Kingdom
"Discriminant Analysis"
Ian Cowe, Scottish Crop Res. Institute, Scotland
"PROSPECTOR: Principal Component Analysis of NIR Spectra" Harald Martens, Norw. Computing Cntr., Oslo, Norway
"Soft Multivariate Calibration with UNSCRAMBLER"

AUGUST 16 - TUESDAY EVENING

SESSION 5 (7 PM): *Spectroscopy of Water*

Chairperson: Dr. Robert Windham, ARS/USDA, Athens, GA

Phil Williams, Canadian Grain Commission, Winnipeg, Canada
"Influence of Temperature on the Spectra of Water in Cereals"
Ian Murray, N. Scotland College of Agriculture
"Interpreting the Spectra of Water"
Paul Mathewson, Nabisco
"Correlation of Water Spectra in the MIR and NIR" Steven Delwiche, USDA/ARS, Cornell University, Ithaca, NY
"Effect of Temperature on the Spectra of Water"

| August 17] WEDNESDAY MORNING

SESSION 6 (8 AM): *Diffuse Reflectance Infrared Fourier Transform Spectroscopy*

Chairperson: Peter R. Griffiths, Univ. of Calif. Riverside, CA

E. H. Korte, Institute of Spectrochemistry, Dortmund, FRG
"Diffuse Reflectance Infrared Spectroscopy of Non-particulate Samples" P. R. Griffiths, Univ. of California, Riverside, CA
"Diffuse Reflection from Inhomogeneous Samples" Robert G. Messerschmidt, Spectra Tech Inc., Stamford, CT
"Diffuse Reflectance Infrared Spectroscopy- Photometric Considerations"
J. J. Venter and M. Albert Vannice, Penn. St. University University Park, PA.
"Characterization of Carbon-Supported Metal Clusters Using DRIFTS"
J M. Olinger and P. R. Griffiths, Univ. of Calif., Riverside, CA
"Quantitative Comparison of Diffuse Reflectance Spectra of Wheats in the Near and Mid- Infrared" R. M. Hammaker, Robert Freeman, Allan P. Bohlke and W. G. Fateley, Kansas State University Manhattan, KS
"Hadamard Transform Spectroscopy for the Near Infrared Region"

AUGUST 17 - WEDNESDAY EVENING

SESSION 7 (7 PM): *Standardization of Instruments*

Chairperson: Mr. K. H. Norris, USDA, Beltsville, MD

Edward Stark, KES Analysis, New York, NY and K. H. Norris, IRL/ARS, Beltsville, MD
"Measuring Wavelength Parameters in NIR Spectrophotometers" **Dave Funk, Federal Grain Inspection Service, Kansas City, MO**
"Standardizing and Monitoring a National Network of NIR Instruments for Protein Analysis of Wheat"
John Shenk, Agronomy Dept., Penn State University, University Park, PA
"Using Software to Standardize NIR Instrument"

[August 18] THURSDAY MORNING

SESSION 8 (8 AM): *New Hardware in Diffuse Reflectance Spectroscopy*

Chairman: Dr. Philip C. Williams, Canadian Grain Commission
Winnipeg, Canada

Bran+Luebbe	- Gabor Kemeny
Labomim	- Dr. F. Kulcsar
LT Industries	- Isaac Landa
Oxford Analytical	Instruments LTD.- Tony Davies
Pacific Scientific	- Don Webster
Percon	- Sammy Gabriel
Tecator	- Terry Hershel
Trebor	- Bob Rosenthal

I AUGUST 18 I THURSDAY EVENING

SESSION 9 7 PM): *Banquet*

Speaker: William G. Fateley
Kansas State University, Manhattan

August 19 - FRIDAY MORNING

SESSION 10 (8 AM): *NIR Band Assignments*

Chairperson: David Honigs, University of California
Washington, Seattle, WA

D. S. Himmelsbach, USDA/ARS, Athens, GA
"Employment of NMR and FT-MIR Spectra to Assist in Band Assignments of NIR Spectra" Ed Stark, KES Analysis, New York, NY
"Temperature and Salvation Effects in Water" Jim Callis, University of Washington, Seattle, WA
"Use of Band Assignments to Develop Calibrations jar Ions in Aqueous Solutions" Emil Ciurczak, Coll. of St. Elizabeth, Convent Station, NJ
"General Correlation Charts for Compounds in the NIR Region" Gabor Kemeny, Bran+Luebbe, Elmsford, NY