Karl Norris, The Father and Founder of Near-infrared Spectroscopy

Introduction

Karl Norris has left us, and the World of Near-infrared Spectroscopy will never be quite the same as when he was with us. A number of his colleagues have sent their personal memories of him, and their comments will be posted, in alphabetical order, in the form of a commemorative folder, on the CNIRS and ICNIRS websites, to coincide with the time that they would be making them as presentations at IDRC-2020, which, regrettably, will not take place at the end of July this year, as originally scheduled.

Contribution by Woody Barton

Commemorative Karl H. Norris
May 23rd, 1921 - July 17th 2019

This tribute to Karl will truly be a test of memory. I began graduate studies more than 50 years ago and became aware of Karl Norris in the late 1960's (**Slide 2**). My dissertation was a kinetic study of extra electron species and the analytical technique utilized NIR (SWNIR) and Least Squares statistical analysis. It was not quite equivalent since I was looking at the spectra of electronic transitions, not vibrational ones. The former being at least 10,000 times more intense, so very thin cells and pathlengths. The calculations were made by carrying boxes of 80- column cards to a building on campus and using an IBM 1620 which took up all of a 14' X 14' room. **Slide 3** gives some references to Wilbur Kaye and Karl Norris that I was aware of at that time. It was Tony Davies who made me aware of Herschel's work some years later and gave the name Herschel region to SWNIR.

After graduation and active duty in the US Army I joined the U.S.D.A. Agricultural Research Service (ARS) in 1971. My job was to study the composition of forages to benefit ruminant nutrition and aid Agronomists and Animal Scientists. Around 1972 I was asked by my supervisor, and this is as close to a quote as I can remember, "do you know anything about NIR"? I said Yes and was sent to see Gerry Birth and Dick Leffler, **Slide 4 and 5,** four floors up in the Russell Research Center. We talked, and Gerry told me about his time in Karl's laboratory. Shortly after that a visit to Beltsville was made and I met Karl, about the time the photograph in **Slide 6** was taken. I got a Neotec FQA51A (**See schematic and spectra in Slide 7 and 8**) and began developing models for forage analysis. The FQA51A had enough of a spectrum to use chemometrics. It wasn't as good as the Cary 14's being used by Karl and Gerry, but a place to start. I then met John Shenk (**Slide 9**) who was working at Penn State and had a Jobin-Yvon monochromator and small mini-computer and did the initial forage study with Karl. I also met Fred McClure (**Slide 10**) at NC State Univ. who had built a system with a Cary 17 and Data General mini-computer.

This group along with Wilda Martinez, ARS, National Program Staff, decided to form the National NIR Forage Research Program at six locations. State College, PA, with John Shenk and Mark Westerhaus where temperate grasses and haylage were studied, as well as software developed, was the first location. The second was the ARS laboratory of Karl Norris in Beltsville, MD, where the

engineering expertise resided. The third location was the ARS laboratory in Athens, GA where Bob Windham and myself were located studying warm season forages and livestock systems. The fourth location was the ARS facility in El Reno, OK, where the Southwestern livestock systems and prairie grasses could be found. The fifth location was the ARS laboratory in Minneapolis-St. Paul, MN where temperate grasses and dairy cattle were the focus of research. The sixth location was the ARS laboratory in Logan, UT where Western grasses and livestock were the research focus. These six locations covered the breadth of the U.S.A. and the grasses prevalent in each area. Funding was obtained for six instruments (**Slide 11**). I do not have any photographs of the early computers. Prior to the DEC Vax 2000 in **Slide 11** we used DEC PDP 11-03's, PDP 11-34 and VAX 11-750 in my laboratory. As they say the rest is history.

This group stayed together for almost 20 years. We met and argued and made great strides. In one early meeting John Shenk wanted a name for the application of statistics to the NIR spectra. I said Bruce Kowalski had coined the term Chemometrics for the use of multivariate statistics to extract chemical information from spectra. I was nominated the group Chemometrician, a role I have tried to live down as I am still learning. At another meeting Karl was showing spectra he obtained for oilseeds and noted that there was always a double peak at 1730 nm and 2315 nm. I offered that they were the symmetric and asymmetric C-H stretch of the combination and overtone of the fundamental bands from the mid-IR. I got the job of spectroscopist for that one.

We found out NIR analytical work was much better than our wet chemistry and it helped us reduce the errors of our wet chemistry methods and thus the NIR RMSEP. So, what did all this working closely together for so long give me from Karl? It gave me an appreciation for the need of protocols. This began when Karl and Wilda got me to be on the AOAC Editorial Board with the goal of undertaking collaborative studies to get "Official Method" status for NIR. This we did for Protein, ADF and Moisture, the later with Bob Windham as Associate Referee. Karl stressed the need for precise language and instructions and I found out that smart people can really mess up simple instructions. I had three pages of instructions on how to dry crucibles and get weights. We had to disqualify one laboratory for their innovative interpretation which put their error way outside the rest. I remember the famous talc experiment. Our task was to take the spectrum of a series of talc samples. The instructions were 15 pages in all. I was reminded of my 4th grade math teacher who wanted us to show all 14 steps of 6+4=10. Karl was meticulous and it has greatly benefitted me in how to generate data sets. The other thing I got from Karl was the desire to make models as simple as possible (preferably one term). We shared an understanding of "make the measurement at the best S/N you can and try to find those wavelengths that were selective for the analyte". In my graduate work I could use a single wavelength and the molar absorptivity to calculate concentration. We will never get there for agricultural materials, but striving for it is a worthy goal. The culmination of the Network's work was Handbook 643 (**Slide 12**). In the late 1980's it was the definitive work on Agricultural NIR and in two editions and 14,000 copies, a well-received document.

There are two other aspects of Karl's work which impacted my own. One was the quest for an immutable standard. The afore mentioned talc studies were one of those efforts, The use of rare earth oxides another. I tried to encase forage in a plastic. We tried to use styrene so that it would be in a hydrophobic medium, but the forage contained too many free radicals and styrene would not polymerize. We even got NIST to help and they could not get it to work. We could get it to

polymerize in the same materials used for Electron Microscopy, but the plastic took in and released moisture to a greater extent than the forage. We are still looking for that immutable standard. The last item to mention is water. It is the one required assay for which there is a molecular weight and one that is so hard to do properly. The Rime of the Ancient Mariner was correct (whether Rhyme as in poem or Rime as in frost) water, water everywhere and no one measures it correctly.

Karl was a remarkable sounding board and when the group discussions got heated could always suggest an experiment to resolve the issue. Since I have already stated the length of some of Karl's protocols it was in our best interests to resolve the issues without a lot of new work. There was a method in all those protocols. They made you think about each step and where error occurs. I truly miss those discussions. We say that a major part of IDRC is educational and I remember the zeroth IDRC in 1977 in Athens, GA. Gerry Birth and Karl got William H. Venable to attend and he presented the Misty Pickle Meter. Today it still is the best explanation of a complete study I have seen or read. The last slide (**Slide 13**) is a summary of Karl's achievements, at least the ones that I believe he would cite.

Karl, I hope you enjoy this.

Woody Barton

Commemorative; Karl H. Norris: Slides.

Slide 2. The earliest photo I have of Karl from around 1968

(Slide No. 1 was an Introductory)title slide

Slide 3. W. Herschel, Phil.Transactions of the Royal Soc. of London, 90, 255-283, (1800)
W. Herschel, Phil.Transactions of the Royal Soc. of London, 90, 284-292, (1800)
W. Herschel, Phil.Transactions of the Royal Soc. of London, 90, 293-331, (1800)
W. Kaye, Spectrochimica Acta, 6, 257=287, (1954)
W. Kaye, Spectrochimica Acta, 7,181-207, (1955

W.C.C. Kaye and R.G. Devaney, J. Opt. Sci. Am. 41, 658-664 (1951)
K.H. Norris and W.L. Butler, IRE Trans biomed. Electron., 8, 153-157, (1951)
K. H. Norris, Trans. A.S.a.E., 7, 240-242 (1964)
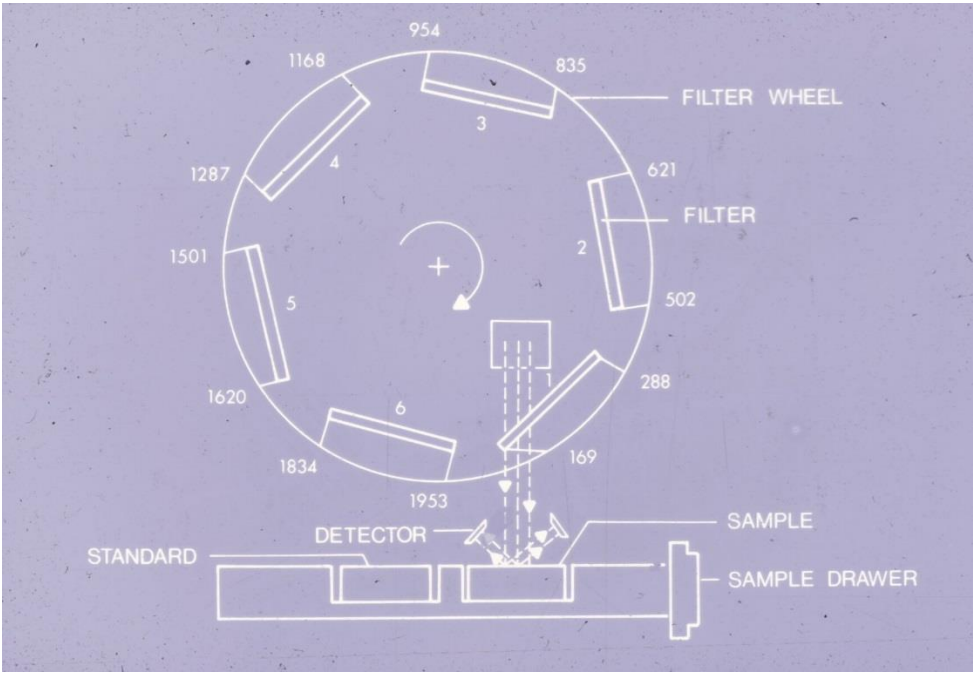

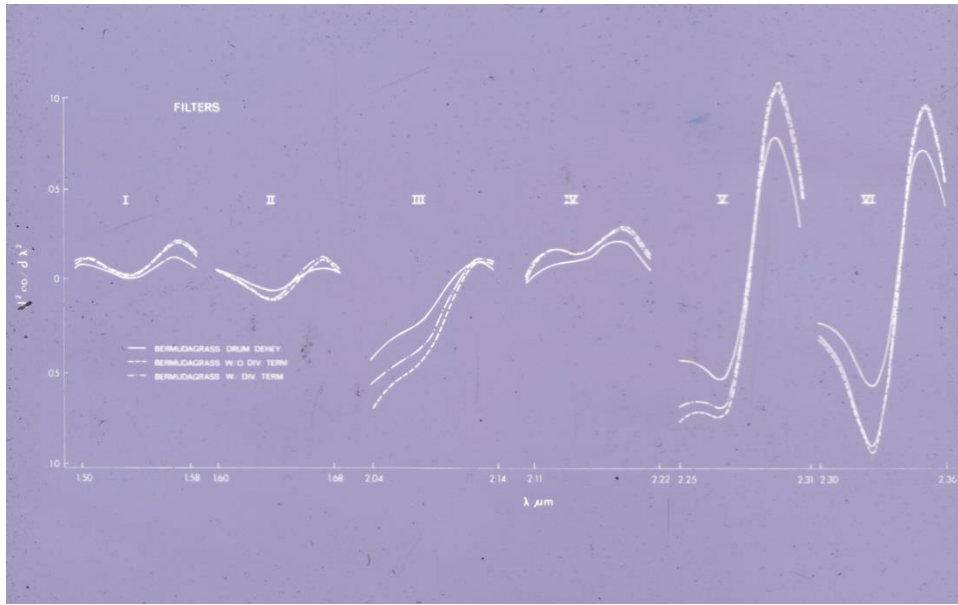Slide 4. Dr. Gerald S. Birth

Slide 5. Dick Leffler with Data General and Cary-14 System

Slide 6. Karl with his Cary 14 Vis-NIR spectrometer

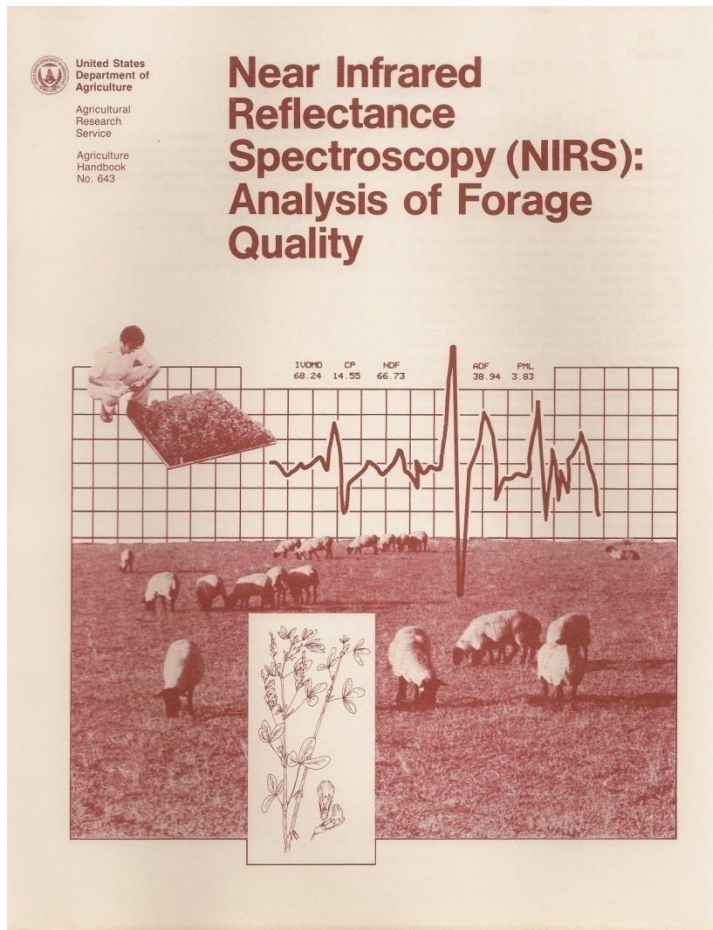Slide 7. Filter instruments

Slide 8. Spectra

Slide 9. Dr. John Shenk

Slide 10. Fred McClure with Data General and Cary-17 spectrometer

Slide 11 National Near infrared Network Instrumentation

United States Department of Agriculture

Agricultural Research Service

Agriculture Handbook No. 643

Near Infrared Reflectance Spectroscopy (NIRS): Analysis of Forage Quality

IVDMD	CP	NDF	ADF	PML
68.24	14.55	66.73	38.94	3.83

Slide 12. First Printing

2000 copies (1984)

Second Printing

4000 copies

2d Edition 8000 copies(1989)

Subsequently translated into seven languages

Slide 13. Karl H. Norris: An interesting career

B.Sc. degree in Agricultural Engineering from Pennsylvania State University in 1942
Doctorate (honorary) from Wilson College, Chambersburg, PA in 2006
Early work with candling of eggs even caught the eye of President Dwight D. Eisenhower
Moisture in soybeans and protein in wheat would serve as a model for all his subsequent work
Worked with the National NIR Forage Network. (where I met Karl)
An abiding interest in developing medical applications for NIR
Long relationship with NIST and metrology organizations worldwide on Standards for NIR

Woody

Contribution by Nanning (Nancy) Cao

In Memory of Karl Norris
May 31, 2020 Nanning Cao

I came to Iowa State University in 2009 to start my Ph.D. study with Charlie Hurburgh, and attended IDRC 2010, where I met Karl for the first time. As a graduate student researching on NIRS, I was so excited to meet "the Father of NIRS", about whom I had learned for a long time from books and literature. I still remember clearly that he asked about the research I did in China and was very happy to discuss his work on the fourth-derivative with me. He had such a sharp mind and his passion of spending all his lifetime on NIR research really inspired me at that young age.

Karl also showed up in the following IDRCs. He even told me one time while we were waiting in line for lunch that he drove to Chambersburg himself in his 90s. After those years, I've graduated from my Ph.D. and came back to IDRC as a young professional. Then, every time I saw those graduate students that were taking pictures with Karl for the first time, I felt that I saw myself in 2010. Karl was a legend and the technique he invented is applied in all kinds of industries. He will never be forgotten by all of us that he had a great impact on. As the president-elect of CNIRS 2020, it is my privilege to continue what Karl has started to the new era. Deep in my heart, he will always be my mentor in science.
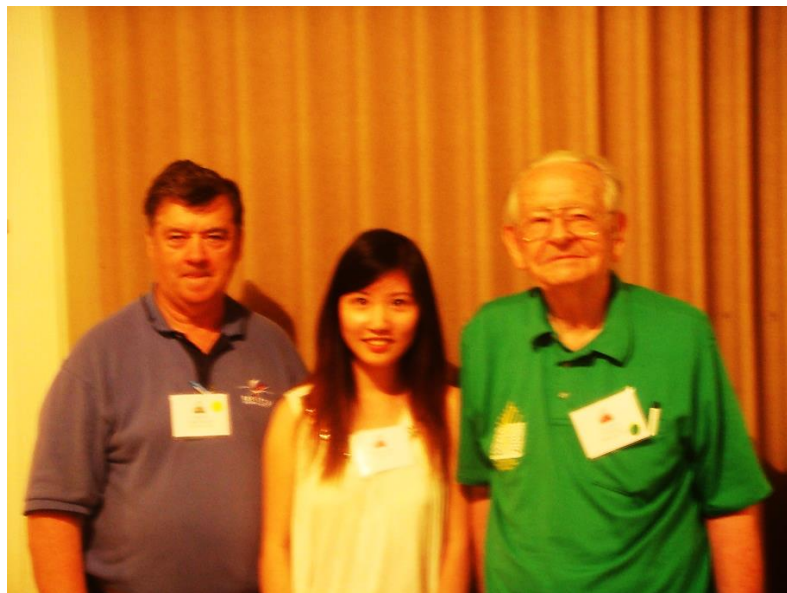
My first-time meeting Karl at IDRC 2010 with Phil Calvi

Contribution by Emil Ciurczak

Memories of Karl

My first introduction to Karl wasn't a formal meeting; it was more of a "teaching moment." I was in the second year of "playing with" NIR (1984) and was presenting some results at the Technicon meeting. They were nice enough to make my slides, so I hadn't seen them prior to the meeting.

So, I hastily went through them and placed them in some order in the slide carousel, immediately before I was to present them.

My project was performing thin layer chromatography, using NIR as the detection method. I was "inspired" to see how small an amount of analyte could be seen, since the Technicon salesman insisted that one could not detect/analyze less than 0.1%. I wanted to see if I could detect and quantify microgram amounts. Using benzoic acid and thiourea in amounts from 10 to 45 micrograms on silica TLC plates (Figures 1 and 2), I showed that, indeed, one can see that level of analyte.

However, in my enthusiasm to show that "something happened," I overlooked a few basics. I pointed to the slide (Figure 2) and showed that the peak differed, corresponding to the amount spotted. In my haste to move along, I simply stated, "The peak seems to diminish as the analyte increases, but I'm not sure why." [Remember, I had only been doing NIR for about one year, at that point.] At that point, a distinguished-looking gentleman stood and said, "That's the water peak. Your analyte is covering it up." While I was nonplussed at the time, looking back, I am grateful that Karl stopped there… Had I been he, I might have added, "stupid!" However, he was as gracious as he was intelligent.

I actually didn't "meet" him until several years later (1987 or 88) at an AACC meeting in St. Louis, MO (in muggy July) when I was consulting for Technicon. He was presenting for Pacific-Scientific in a joint two-vendor exhibition with us (in the same room). I was too engaged in listening to his presentation to notice the condition of the Technicon instrument (that I was to demonstrate) as it was delivered.

The staff at Technicon did not send it in the proper container, but simply a cardboard box, filled with polystyrene "peanuts." As you would imagine, the box fell apart as it was placed on the table, spilling the packing materials on the floor. Adding to my woes was the fact that the instrument was missing a leg (which I replaced with a soda bottle cap), was equipped with a fiber optic probe (with which I had never worked), and was being run by a new model computer (that I had never used) with some updated software (of which I didn't recognize some functions).

Just as I realized that they didn't pack the sample cups, Karl walked up and introduced himself (mercifully, he either forgot my *faux pas* of a few years earlier or was just being polite and didn't mention it). He was carrying a number of small plastic bags filled with white powder. After I showed him the instrument (allowing time for warming), He asked if I could measure the "hardness of wheat." While my mind said, "What the heck is 'hardness of wheat'?", my mouth said, "Of course."

As Karl asked for the sample cup (which I didn't have), he spurred me to my first methodology "discovery." I looked him in the eyes and calmly said, "We don't need the cups, we can use the fiber probe (reflection-type) and read directly through the bags." Somewhere in the back of my mind, I was thinking how I just lied to the King of NIR without blinking. To make a long story short, *it worked* and I've been working through plastic since.

I was always grateful that, at almost any meeting where I presented, I could depend on Karl be sitting near the front of the room and waiting to ask the best question of the group. I used to tease him (and, rest assured he laughed with me) by saying things like, "I see Karl out there; a man I consider in the twilight of a mediocre career." He always told me after the session that he enjoyed my wit. One time, after being lectured by the wife of another researcher that I needed to be more professional, I presented a paper without humor of cartoons. After which, Karl came up to me and said, "Good results, but it was the most boring talk you ever gave… and, you didn't mention my name once." Of course, I was never serious again.

Years later (1998), I was fortunate enough to have Karl work on matching two NIRSystems units for my work in pharmaceutical tablet transmission analysis. The two were so well-matched, I never needed a bias or skew adjustment AND, the spectra generated were interesting enough (and novel enough) for Karl to use them in his talks for years to come, always squeezing out one more iota of information, each time. I beamed every time he pointed out that the spectra were generated by Gary Ritchie and me.

Karl always had time to sit with me and answer questions (some of which I hadn't even asked) as in Figure 3. But my proudest (if not somewhat sad) moment came when I was tasked with putting together a session at Chambersburg, a few meetings ago. Since it was after the Sunday dinner, meaning a combination of full bellies, wine, and travel weariness, it needed some "pizzazz." I filled it with old-timers and named the session, "What we did before the Internet." Of course, Karl was at the top of the list, as well as Lois Weyer, Howard Mark, and Phil Williams.

When I contacted Karl, he asked if I could put his slides together from some loose pictures, because his memory wasn't as good as it used to be. I obviously accepted the honor (although he considered it a task for me) and set about doing my best. Later, after I sent him a copy, he asked if I would mind actually presenting the slides in his place. I chewed over the answer for 10-15 microseconds and accepted the "chore."

As I gave the talk, I considered how far I had come in the science of NIRS. After stumbling into the technology in 1983 (we needed a fast way to qualify raw materials at Sandoz), giving a so-so presentation and being verbally "spanked" by Karl for a rookie error, actually performing some reasonable work, being honored by Don Burns as co-editor of his Handbook of NIR, having the great Karl Norris use some of my data for his work, and eventually actually presenting *his* accomplishments, using *his* pictures and data, in a slot that was designed for *him*, I finally felt that I had finally arrived into the "fraternity" of NIR users.

I have nothing but admiration and love for Karl and miss him personally as well as professionally. I am most pleased that he got to see the third edition of the Handbook dedicated to him. Rest in peace, *Sensei.*
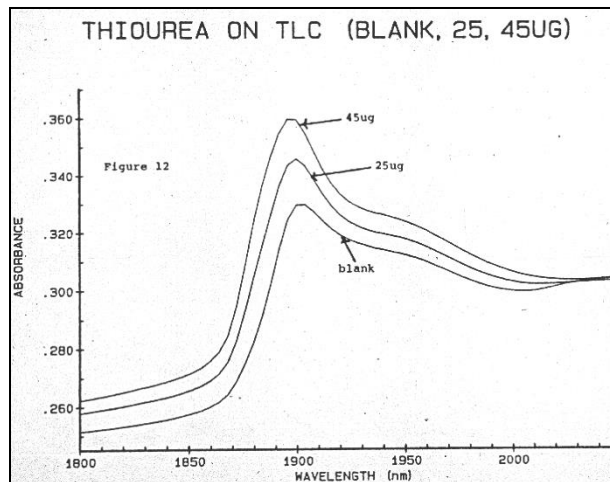
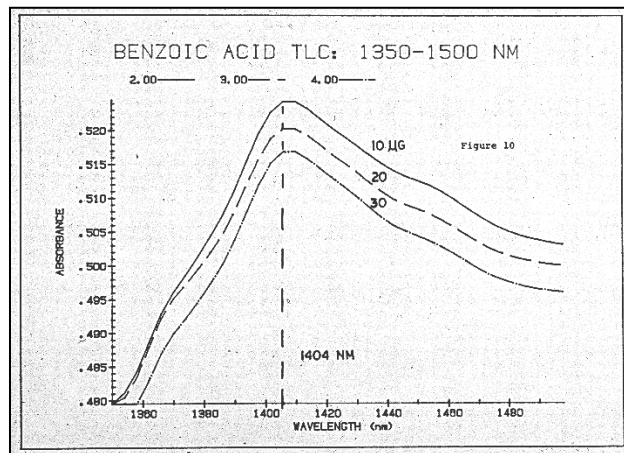Figure 1. Blank plate, 25 and 45 micrograms of thiourea spotted.

Figure 2. 10, 20, and 30 micrograms of benzoic acid on TLC plate.

Figure 3. Learning from two masters; Drs. McClure and Norris.

Contribution by Don Dahm

Karl Norris and the Representative Layer Theory
Donald J Dahm

It is no secret that those of us who knew Karl love talking about our interactions with him. We often measured the importance of our own contributions by his opinion of them. It is impossible for me to separate our interactions involving science from those that were personal. Everything he did was permeated with thoughts of near infrared spectroscopy close by. He described himself as addicted, and I said that I too was hooked, and predicted that I would never leave the field.

It's been about 35 years since the publication of Phil and Karl's <u>Near-Infrared Technology in the Agricultural and Food Industries</u>. I myself am now an old-timer, even though I am clearly not one of the founding members of the field. (I was told by a beautiful, young French woman at NIR-2013 that I was the third oldest person at the conference. Probably not one of her better pickup lines!) Perhaps I could tell you how I became involved in the field of NIR and eventually with the publication of the second edition of said Handbook. But the main point of all this will be to describe how Karl Norris contributed to the development of Representative Layer Theory, which came to pass after theoretical work in the area of Diffuse Reflectance had languished for many years.

I entered the field of NIR spectroscopy by becoming an employee of NIRSystems. I wanted to once again be a practicing scientist after a lucrative career ending in being jettisoned from an upper management position at age 50. I had been trained in a highly mathematical field as an X-ray crystallographer. That field had passed me by, and the chemometric nature of NIR analysis was attractive. I knew little about the field, but was anxious to learn. A few weeks into the job, I overheard someone complaining about a software problem in an adjacent room. When he left, I asked "Who is that old man?". "That's Karl Norris." The way it was said kept me from asking what I wanted to know: "Who the hell is Karl Norris?"

Well, as far as I could tell, he was the only guy in the place who really paid attention to the science of things, so I began to visit him in his office. (Still didn't have a clue who Karl Norris really was. Just trying to soak up some understanding.) I would ask him what he was doing and why. (I was just asking questions, the kind a research director asks when he reviews projects.) Sometimes he would say something like: "That's a great idea; I'll give it a try". (It's possible he was just being nice, but I think that my questions sparked ideas in him that he incorrectly attributed to me.) At some point, I got brave enough to ask a question that would expose my lack of knowledge.

I had just collected data on two samples. One was on a powder; the other on pellets extruded from that powder. The pellets gave a very strong {log(1/R)} signal; the powder had a pattern barely discernible from the background. I reasoned (not correctly) that the samples were the same except the pellets had a larger void area in the sample, and since all I was doing was reducing the amount of sample per volume, I would reduce the α and σ proportionately, and the ratio should remain constant, implying no change in absorbance. I wanted to know why the absorbance metric was so strongly affected.

Karl explained to me that it was due to a pathlength difference. That was my first exposure to what I've come to call his Intuitive Model. (I've included an illustration of the model. The ideas were Karl's; the drawing is mine.) His idea was that as either absorption or scatter went down, the sample penetration would go up, yielding a longer pathlength. In this case, both the absorption and scatter went down due to concentration, but scatter also went down due to the fusion of particles during the extrusion process.

Effective depth of penetration into sample
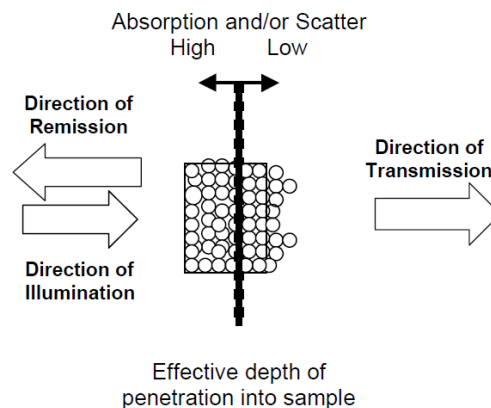
While that was impressive enough for me, he went on to say that he trusted no theories that did not include pathlength, and that I should be reading the theory in the "Ag and Food Handbook" instead of the Handbook of NIR Spectroscopy, and he loaned me his copy. There I was exposed for the first time to *The Physics of Near-InfraRed Reflectance* chapter by Gerry Birth and Harry Hecht. While there was plenty of math there, there were pictures and charts that appealed to the eye and intuition rather than the brain. I was a changed man.

In 1996, I attended my first IDRC. It was here that I first realized what a god-like figure Karl was to so many people. Karl gave two talks:
Diffuse Reflectance Spectroscopy: 1) Where Are We and What Needs to be Done?
                                                            2) How Should We Treat the Data?
At the first talk, which was the keynote talk, Karl opined that the theory was lagging behind the chemometrics and there was a need to catch it up. In the discussion following the second talk, I wrote out the general form of the mathematical solution. I also gave a poster, which did not disclose the math, that explained why the $\{\alpha/\sigma\}$ thing was incorrect. (Gerry Birth seemed to be the only person who understood the significance of what I was saying, but unfortunately he was no longer comfortable carrying on a discussion with anyone but his son.)

After hearing in confidence where the math stood, Karl persuaded Don Webster (NIRSystems president), in exchange for any patent rights which might exist, to give me a grant to work with Karl in the NIRSystems facility to develop the mathematics into a usable theory. After a period of "thrusting around", we sat down one day and Karl described all the generalizations he could recall from the data he had collected over the years. (He seemed to remember every experiment he had ever done.) Next we developed a list of questions which the theory should explain. (For example: Why are small particles "over-represented" in the absorbance spectra?). … Then Karl gave me what I blasphemously referred to as "the great commission". He wanted to understand the theory well enough to answer these questions before he retired.

When I finally came up with the Representative Layer Theory, Karl was bothered by the fact that the layer was a different thickness at different places. He thought I needed to describe how these layers fit together to fill space. In a spirited discussion, I took a bottle of particles, repeatedly shook it and gingerly put it down (I'm trying to avoid the word "slammed") on the table. I said: "Each time I shake it, the bottle has a different void fraction, which is what contributes to re-pack variation in spectra. Aside from that, the representative layer is identical in each. I don't have to

tell you how the layers fit together in each; it's enough to know that God was able to do it." I knew I was winning the argument when his scowl was replaced by a smile. I almost always curtailed our arguments, because if I wasn't sure of my position, I would quickly yield to his vast experience and knowledge before a real argument started.

One area where I should have argued more was on the issue of whether there is a single scattering coefficient for a sample, or whether the scattering coefficient changed with absorption. I spent weeks, without success trying to extract that single coefficient from a set of data Karl had collected from a set of plastic sheets. Karl then got a paper from Thorsten Burger ("Diffuse Reflectance and Transmittance Spectroscopy for the Quantitative Determination of Scattering and Absorption Coefficients in Quantitative Powder Analysis") which agreed with my position. Karl said he owed me an apology, but I refused to hear it. Just told him I learned a lot that I needed to know in the process of chasing his idea. Eventually, Karl came to believe that the theory was in pretty good shape, and suggested it be me that would update Gerry Birth's and Harry Hecht's Physics chapter for Phil's and his handbook. (Just so you know, Karl very much let Phil do the project's heavy lifting.) The only guidance I got from Phil was to make damn sure that the color photos from the first edition remain in the chapter.

 As we were working, we became convinced that the best single measurement to make on a powder was on a thin sample in transflectance. This bothered Karl because he had frequently gone on record saying that the best sample for reflectance measurements was an "infinitely thick" one. He asked me to develop the mathematics to relate the apparent absorption coefficient observed in transflectance to the one that would be observed in transmission. With Kevin's help, we did so, and published it: Donald J. Dahm, Kevin D. Dahm, Karl H. Norris; Obtaining Material Absorption Properties from Remission Spectra of Directly Illuminated, Layered Samples. I don't remember much about the paper, probably because I was between jobs and wives while it was being written, flitting around the world (literally). Karl never wanted his name on anything unless he had collected data for the study, and then he always wanted his name last. (I know my name appears first, but credit this one to Karl and Kevin.)

In 2005, Karl was the session chair and presenter at the EAS Award for Outstanding Achievements in NIR / Vibrational Spectroscopy for our work.

I was able to arrange for Karl to receive an Honorary Doctorate from Wilson College in 2006. It was given at the IDRC banquet. Karl (and most of the audience) didn't know it was going to happen. Susan Foulk pulled Karl out into the hallway, and dressed him in his robe. I just said: "This is for real. Smile all you want to, but don't laugh." That was the only time I ever heard 'Pomp and Circumstance' played on guitars.


Some things Karl told me that you may not have heard: He had begun college hoping to become a designer of agricultural machinery. But WWII intervened. … He met his wife though letters she was writing to various soldiers. … He got into NIR because, when he suggested at an inter-

departmental meeting that it may be ideal for a problem at hand, the analytical chemists pretty much ignored his suggestion. ... He made sure that contracts for the building of an instrument were given to different groups so as to create competition. ... He always kept his personal copies of software separate from that of NIRSystems, and complained when they labeled something that departed from his method as "Norris Regression". … He wouldn't be leaving the USA anymore because of his wife's health. … His memory of past experiments was fading.

The last time we argued was in print on the NIR Discussion Forum (I kind of forgot we were "in public"). He wrote in response to my criticism (about something that turned out to be more of a misstatement than a misconception): "I hope those who follow this discussion are aware that Don and I have been co-workers and good friends for a long time. I think we make a good combination with Don focusing on the theory, while I focus on the experimental data. We don't always agree and we don't hesitate to say so."

I was honored to be numbered among Karl's many friends.

Photos of Don Dahm used as a slide for Birth Award Talk at IDRC in 2014.
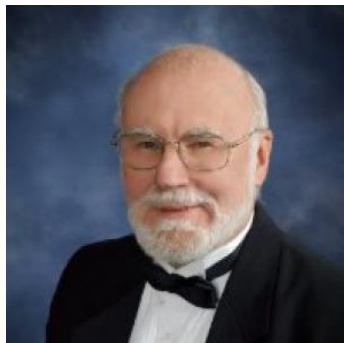
Captioned (by a student) on a fake Twitter feed: "I don't always wear this hat, but when I do I'm high …., and talking about dwarfs."

I assure you. It's only caffeine!

Contribution from Tony Davies

Karl Norris
Tony Davies, NNIRC.co.uk
10 Aspen Way, Cringleford, Norwich NR4 6UA, UK

I'm sure that we all remember our first meeting with Karl. I certainly do! It was at the first IDRC meeting at Wilson College, Chambersburg, in 1982. This was my first trip to USA and my first experience of "jet lag" and I was not sleeping well. On the first day of the conference I woke early and went for a run and looked forward to meeting Karl Norris. I didn't get a chance; he was always surrounded by other delegates, with the same intention. I woke early on the second day and started out on my run but after a few minutes I caught-up with Karl on his morning walk ALONE!! I instantly decided that I wanted to walk and we had a lovely chat for about twenty minutes. When I returned to my room I realised that he seemed more interested to learn what I was hoping to do with NIR than discussing what he had done!

I made several visits to Karl's lab and in the first few years he was developing his NIR method for measuring human body fat. He called me "our lean standard" (which greatly pleased me!). On one visit he said "We are giving a demonstration of the method to the Secretary of Agriculture's Advisory Committee. Would you like to come along?" "Yes please ". The Secretary's committee was "PC" at work. Three women and two men one of them black. Karl described the instrument and demonstrated on himself and then asked them "Would one of you like to try it?" After a moment's pause the black man stepped forward. "Yes, sure", rolling up his sleeve. Karl was clearly embarrassed. "I'm sorry but it doesn't work with black skin … but we are working on it"! Another pause and then one of the other four members step forward saying "Try me". Karl selected one of the ladies and all was well. The lean standard kept quiet!

Karl loved to surprise people. I once opened a letter from him and found he had sent me his first NIR spectrum! It was of a newly laid chicken's egg; he was trying to find a measurement for "freshness". It had taken 10 minutes to make the individual measurements of each point in the spectrum, at 10nm intervals, by carefully adjusting the spectrometer. There was a set of spectra taken at 20-minute intervals, which clearly showed a change with time. For a short while Karl thought that he had made a discovery but after further thought he realised that what he was recording was the egg drying out in the first hour or so of being laid. He had put them away in a file and they had been in his filing cabinet for 40 years! He thought I might be interested. It was the first "scoop" for NIR News!

In 1983 my group at the Food Research Institute became interested in work done by Tom Fearn on the "best-pair" of correlating wavelengths for determination of an analyte in a particular sample type. If the spectrometer measures absorption for every second wavelength over the range 700 to 2400 nm then there will be 244,650 possible pairs (which even in the 1980's could be computed quite rapidly by a micro computer) but this is only the beginning of the search. We decided on a colour-graphic approach which allowed an operator to select promising areas for additional computation. I presented our method at a meeting in Washington in 1984 but I didn't think Karl was interested or impressed. I was able to visit Karl's lab in August, 1984, (on the way to Chambersburg for the second IDRC) and after Karl had discussed some of his work he said "we

have something to show you. We thought your colour-graphic method was interesting so here is our version" and he showed me something similar to CROME but then he said "we have a new computer so we thought we would see what it could do". He then showed a second program which computed areas of interest in real time! I was amazed, our programs required two over-night runs to produce our results (close to 30 hours of computing!). I once did manage to surprise him. At the 1997 ICNIRS conference in Essen, Germany we made Karl the first Fellow of Near Infrared Spectroscopy and as well as the plaque I presented him with a Special volume of JNIRS in his honour, which we had managed to produce without his knowledge! (Photo 1.)

In 1998 the Analytical Division of the Royal Society of Chemistry announced a new prize with an unusual specification that the nomination should be for the developer or co-developer of a significant advance in analytical chemistry, the recipient could be of any nationality and need not be a chemist. The prize to be called the Sir George Stokes Award and the recipient will receive a medal. (It is often referred to as the Sir George Stokes Medal). When I read about it I thought that Karl should be the obvious choice for the first award in 1999 but I was disappointed that it went to Alec Jefferies, for DNA profiling (a good choice but I thought the first award ought to have gone to a non-British subject). I was successful in my bid for Karl to get the second award in 2001 Karl came to London for the award ceremony and I didn't want to miss the opportunity for Karl to give a lecture to the NIR community. With help from Tom Fearn, I organised a meeting at University College London and Karl gave two lectures while Tom and I completed the programme. When we finished Karl said that he was a little tired! I thought, "I hope he will be OK for tomorrow". I should not have asked him to do so much! But he was fine and the audience were obviously impressed; particularly by him telling them that some of George Stokes' more obscure mathematics had been used in his most recent publication with Don and Kevin Dahm! (Photo 2).

Karl was genius, but just as important, he was a very lovely man. He changed many people's lives when he converted them to NIR but he changed mine twice! At the 1986 international NIR meeting in Budapest there was not much support for the Russian proposal for the formation of an international body. It was suggested that a sub-committee should be formed and in addition to the expected names Karl suggested that I should be the UK representative. The sub-committee didn't like the Russian "top-down" proposal but came up with a "bottom-up" idea which was named ICNIRS. The result was that I organised the first ICNIRS conference in 1987, became Treasurer and Secretary (briefly) and later chairman, started NIR news and JNIRS! All because Karl had "elected" me to the sub-committee when I was a very much a new boy in the NIR field!

I am doubly grateful to him and his wonderful beneficial effect on my life.

Figure 1. Presenting Karl with the Fellow of NIRS plaque.

Figure 2. Karl with the Sir George Stokes medal.

Contribution by Tom Fearn

My favourite memories of Karl are of his repeated success, until he disqualified himself to give someone else a chance, in winning the "shootout" spectral data analysis competition at Chambersburg. It was like watching amateurs play against a grand master. When I'm tempted to feel proud of some sophisticated chemometric analysis, I try to remember that Karl would almost certainly have been able to beat my efforts with a deceptively simple regression equation and with a smile on his face. His passing is the end of an era, and he will be sorely missed by the whole community of NIR researchers that has grown from the seed he sowed.

Tom Fearn
Chemometrician and current President of ICNIRS

Contribution by Susan Foulk

Memories of Karl Norris
Susan Foulk, Guided Wave, Inc.

I was a newcomer to NIR spectroscopy back in 1987 when I joined Guided Wave (GWI). I met several people at Tecator and NIRSystems early on and became aware of Karl and his ground breaking work in the NIR field. I first met Karl in 1992 at the Chambersburg Conference and saw his presentation for the first Software Shootout that year. Karl was always willing to share his expertise, and his vast experience was an invaluable resource to the NIR community. It was a pleasure to see his Honorary Doctorate Ceremony at Wilson College in 2006 – a well deserved honor. I enjoyed participating in the Software Shootouts in those early years and I personally benefitted greatly from these events. Karl was a treasure for the NIR community and leaves a legacy for all.

Contribution from Ana Garrido-Varo

In memoriam of Dr. Karl Norris.

Several wonderful opportunities I had to get very close to Karl Norris

I think that I saw Karl for the first time during my attendance at the ICNIR Conference held in Brussels (1990) or maybe Aberdeen in 1991? By that time I had studied his revolutionary paper Predicting Forage Quality by Infrared Reflectance Spectroscopy (Norris, et al., 1976) co-authored with Barnes, Moore and Shenk. That paper opened a big door to an exciting scientific career for many animal nutritionists, such as myself. During the same period, I devoured the best piece of NIR educational literature ever written, the book entitled Near-Infrared Technology in the Agricultural and Food Industries, co-edited by Phil Williams and Karl Norris. I have several favorite chapters from that book, but the collection of spectra contained at the end of the book has always been of a great help. I never imagined that years later, Karl would personally send me this collection of spectra as a donation to our educational project IVPTL-NIRS . The collection is also available at the ICNIRS website for society members.

I kept seeing Karl at every conference, but I would never have dared to talk to him to ask questions. I always saw him as being very busy and I thought that it was not in order to disturb such an important person. I also remember one of the Conferences (maybe in Haugesund, Norway?) that when we were at the gala dinner, somebody asked for silence and we could hear a phone message from Karl. I remember that I was very impressed and moved, and I realized once more, that Karl was a fundamental part of the NIR community. I was emotionally touched by hearing his telephone message in the sepulchral sound of the dining room. No video only voice! I greatly admired his intellectual and human qualities. I have had the privilege of being close to him on several occasions, which I will illustrate with some short comments and photographs.

Córdoba, April 2003 (NIR2003).

I had the great pleasure of having him as a guest at our ICNIRS Conference in 2003. This gave my students the opportunity to learn directly from him (Photo 1). We took the opportunity to interview him in depth, for the largest Spanish daily newspaper, El Pais (Photo 2).

Beltsville , Maryland (USA), March 2007

During a research visit to the Instrumentation & Sensing Laboratory, ISL, USDA-ARS, Belstville, I asked Moon Kim to let know Karl that I would be there for one month. The day after, Karl went to ISL to meet me. He told me that that was the first time he was at ISL since his retirement. I think he enjoyed that day. I took a picture of him in the front of a photo of him taken in the late 60´s, with President Eisenhower attending a demo of Karl's machine for Automatic Detection of Blood In Eggs. (Photo 3). He also presented me to the Beltsville Rotary Club (Photo 4) where he showed me a book with the names of all the presidents from its creation in 1967. His name was there! He was the 4th President (70-71). I had an incredible experience that day!! He took me on a one-day round trip to Port Matilda, because he knew that I would have liked to take the advantage of my visit to the USA, to meet John Shenk. He drove in heavy snow. Maxine, his wife, scolded him because he drove so fast! During the trip he confessed to me that it was the first time that he had visited John's house. It is a pity that the photo I took of the two giants with part of the families is a bit dark. (Photo 5).

Karl and his interest about determination of fatty acids on humans (2011- 2012)

One of my scientific talks with Karl while I was visiting ISL was related to our interest and need, in Spain, of measuring fatty acids in live Iberian pigs (IP). I knew that he had a paper published (Conway, Norris

and Bodwell, 1984), aimed to estimate body composition of humans. I enjoyed very much learning from him how the distance between the source and detector affected depth of penetration into the body. He showed a great interest in our research on Iberian pig ham and fatty acids by NIR.

During the summer time of 2011 we returned to the exchange of info about IP adipose tissue. I suggested to him that he could work with our data for preparing a Lecture (Spectral examination and mathematical pre-treatments), for the first course offered by the IVPTL-NIR. I think that he liked that invitation to act as a teacher, and although he resisted initially, he finally accepted with great interest. We decided that he would do some work for the Lecture using our IP NIR data sets. During the next few months we exchanged files and many interesting thoughts. One day he sent to me an e-mail (Photo 6). The e-mail said "I wish to follow up on the possible detection of body fatty acids by NIR transmission on the ear." I attempted to get your spectra from the fatty acids from the web but I could not access them. I would like to know your wavelengths for measuring the fatty acids, to see if I can find such bands in my ear spectra. We sent him several files and after working with them he wrote "I believe that an interactance probe would be able to detect fat spectra and give information about the feed. A transmittance measurement could work if we could find a spot where the sample is thin enough, less than 5 mm. I am very impressed with your data.

Unfortunately a few months after that, Karl started to have problems with his memory and he told me that some days he was not able to find files in the computer. I wish to share with the NIR community that comment through this document. I am very proud of the value he gave to our IP work and very grateful that he decided to share this innovative idea with me in such an altruistic way. Hopefully one day that idea will become a reality. He deserves it.

Chambersburg , August 2014

Finally, I had the great privilege of presenting Karl with the Inaugural ICNIRS Karl Norris Medal (Photo 7).

Karl, thanks for everything, with love and deep gratitude

Ana.

Photo 1. Karl and the UCO team

Photo 2. The journalist, Karl, and me

Photo 3. Karl with President Ike

Photo 4. Karl presenting me to his Rotary club

Photo 5. Photo 5. One giant (Karl) visits the home of another giant (John)
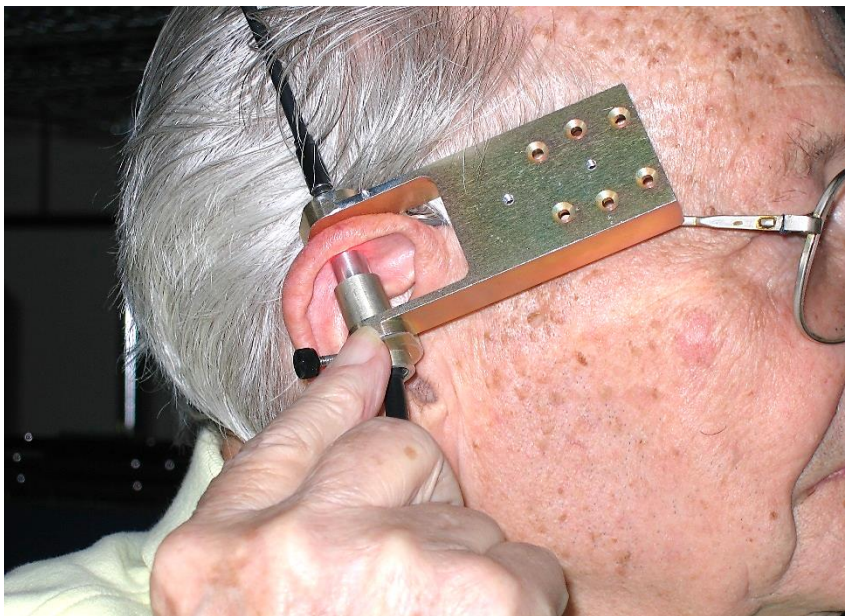For the first time

Photo 6. Karl with the era transmission probe

Photo 7. Karl was 93 years old and Maxine was also attending the award ceremony. Thanks both!!

Contribution by Dave Hopkins

Memories of Karl Norris
David Hopkins, NIR.Consultant @ sbcglobal.net

It is as clear as a movie, we are standing in front of the one of the growth chambers at the Smithsonian Radiation Biology Laboratory, Rockville, MD. It was 1978 and I had invited Karl Norris to bring his own-designed spectroradiometer to measure the lighting in growth chambers I was using to measure the effect of special lighting I set up to mimic ozone depletion on the growth of plants such as peas. While we were standing there, we were chatting. Only as I think back on it now does it seem remarkable, he pulled out from his papers he had with him a NIR spectrum of ground wheat, and announced that a change at 2180 nm the width of the pen tracing reflected an increase in the protein of 1 percent. He knew that from fourth derivative spectra. Well, I had used fourth derivatives to study UV and visible spectra, but the bands we studied were always discernible by eye. I blurted out, "You're crazy!" I regretted it as soon as I said it, but he was gracious to ignore it. He went on to say that he knew of a company in Illinois that was looking for a laboratory manager, and I could write the Vice President of Engineering if I were interested. Well, I did not appreciate that a recommendation from Karl Norris was a shoe-in for the position. I wrote off, and interviewed there. It led to a whole new spectral area and new career for me. At DICKEY-john I met David Funk and a circle of talented engineers. I learned from a number of chemists, and formed a lasting friendship with one of them, Phil Williams. Thanks so much, Karl!

Karl was a master spectroscopist, and it was always a pleasure to meet with him and discuss his latest ideas at the International Diffuse Reflection Conference (IDRC) meetings. I think that the Shootouts were introduced around 1992, and I don't know for sure whether he won them all, but I think by 1998 he had a long string of presentations that edged out all contenders. I remember that Susan Foulk and I pleaded with Karl not to enter the competition, so others could win. Karl took that to heart, and in 2000 Susan remembers that she won, and in 2002 I finally took home the trophy. At that time the winner was honored by presentation by Fred McClure of a simple plastic trophy. I still display that trophy proudly in my office. It was in a way all due to the humility of Karl Norris.

Fast forward to 2015 or so. I knew that the compiled Fortran program Karl used so well, was no longer supported under the DOS window of Windows 7. I phoned him and asked if I could work with him and I would write Matlab programs to perform the same tasks that his MULR program did. He readily agreed. Bill Hruschka wrote the Fortran program, and Karl sent me the latest documentation, a 1998 version of SPANUSER.DOC by Bill, a 1997 version of MULR.exe, all supporting routines and subroutines, and two data files with 50 scans of ground hard red winter wheat each. I would write a version for Karl and send it to him via Internet, and a version for me, because the directory structure of our computers was different. I called it dqm, for derivative quotient math, because he modestly disliked calling it the "Norris Regression" or "Norris Method".

I remember that he loved the speed of the Matlab program, and would chuckle that it was so fast. We set ourselves the task to make the program automatic, so that one did not need to have the tremendous spectroscopic experience that Karl had. I programmed the method outlined by Bill in SPANUSER, and we obtained the same excellent results Bill reported. But Karl wanted to know what would happen if we used a different sequence to optimize the gaps and smoothing gaps

(smts), so I wrote dqm2 and called the first one dqm1. I wrote dqm3 to perform tasks learn about the spectroscopy of the samples, to plot different derivatives to learn the effects of the size of the gaps and smts. Eventually we combined dqm1, dqm2, dqm3 and other tasks into one dqm program, so that the user of a free, compiled version of the program could get the same experience as the user of the Matlab program, which is not free. Because Karl always freely shared his program, I will share the Matlab program freely. David Funk suggested that Zoltan Gillay might compile the program for me. I am grateful to Zoltan for his patient help through numerous versions. Karl and I stayed in contact until a few months before he passed away, but a year or two before that he complained that he could not remember how to use the program, or could not remember how to use his email. It was so sad to witness the decay of his fine mind. I feel very fortunate to have worked with him.

Phil, Karl and I pose at the 2016 IDRC. This picture represents over 250 years on the planet, and about 140 years of experience with NIRS!

Contribution by Christian Huck
In memory of Karl

Meeting with Karl was an experience, from a personal and scientific point of view. First time I met Karl in 2001, Kyongju, South Korea, and I was deeply impressed by his sensitivity in identifying young rising stars at an extremely early time point of their career. In the following years I had the chance to meet Karlat IDRC and discuss with him about several of our ongoing research projects. I was wondering about his patience in listening to my questions and when I asked about his opinion, he knew how to motivate by saying something like "You should do what you want to and how you feel. Then you will know what it means." This was one of the main motivation to continue with our research on nanomaterials, investigating pore diameters being in the Angstrom range. Discussing about Babinet´s theorem he recommended to continue with the experiments. Repeating similar discussions I always had the feeling like coming back home again, being back at the basis. Indeed, Karl always had an open ear for any novel attempts and surprised me with his permanent youth enthusiasm. So I am very grateful that I could have received my take-home message and I like to live the spirit. Finally, there are only a few words left to say to Karl: Thank you, your spirit will always be with us and rest in peace.

Yours sincerely, Christian Huck

Contribution from Charlie Hurburgh
To the NIR Community in memory of Karl Norris

I am sitting in my home office writing this in the middle of a transformational event that history will surely record as life changing for a long time. The university is struggling with the balance of online teaching versus real people using real equipment to teach practical skills. That's where Karl always was…real people teaching about real equipment for real applications.

I tried to send my students and staff to IDRC as much as possible, and I am sure many of you know them, either as students or in their ongoing careers, many of them in the NIR field still…Sylvie, Igor, Nancy, Lidia, Benoit, Connie, Glen and so on. Without question the highlight of their trip, really of their graduate programs, was to be able to meet the person that created the technology that they learned, and who was always their first reference in their introduction. And then to have him take the time with each of them to go through their project in some detail (sometimes more detail, or at least better detail than their major professor did!). I am not sure I know of another situation like that, that lasted over as many years as he and they interacted, much more than the typical one-time symposium or reception. The meaning to those students could not be overestimated.

Personally, I started in NIR totally as a learn as you go situation, with a filter instrument from Dave Hopkins at DICKEY-john, and a lab manager named Lynn Paynter, whom again some of you know. We were asked in 1982 by members of the Iowa Soybean Association Board to look into why soybean prices paid by processors in northern Iowa seemed to be significantly lower than prices paid by southern Iowa processors. The guess was oil and protein levels, and enter Dave, the GACIII six filter unit (which still works by the way), and a bunch of samples. Lynn wore herself out doing extractions and Kjeldahls, and we got a calibration that seemed to work well, at least on these samples from NW and SE Iowa. With six filters, and an ISU mainframe fortran computer that had less power than a smartphone calculating all night (crashing sometimes) there were limits…

The crunch came next year (1983) with a new crop. I still have the printout of the validation; results were only slightly better than the RANDOM function of the then popular breakthrough spreadsheet LOTUS 1-2-3. Lynn cried for an hour. We had the first DOS-based computer in our department, and I blamed Bill Gates. John Shenk said even a low r square had some predictive value. Dave, as I recall, said I should talk to Karl Norris and not give up.

Karl spent more time with us than he probably should have, and probably repeated more of the basics than anyone should have had to. But that was Karl; we left his Beltsville office with several stories and a resolve to try again using his concepts of data-set structuring and in this particular case ratioing the filter values. That was 36 years ago. I have said thank you Karl ever since. Some events, and some people, you just don't forget. Best wishes to all, and Godspeed Karl.

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Charlie Hurburgh, Iowa State University

Contribution from Harald Martens

Karl Norris - Fond memories, deep gratitude and future needs

Harald Martens, bio-chemometrician
harald.martens@idletechs.com

Karl Norris, kind giant

Karl Norris helped us to make sense out of real-world data. He focused on multi-channel data from diffuse high-speed spectrophotometers, primarily in the near-infrared (NIR) wavelength range.

Learning from Karl

Karl helped and inspired me in several ways, over many years. With my background in psychometrics and chemometrics, I was familiar with multivariate data analysis. But as food biochemist I did not have measurements to match it. Around 1980 my friend and mentor in Copenhagen, Lars Munck, sent me to visit Karl in his USDA lab in College Park, Maryland. At that time I had already worked desperately for 8 years to develop methods and tools to extract information from slow chromatographs, to find variation patterns hidden behind lots of rather noisy chemical peaks. Frankly, I felt a bit lonely. But when Karl showed me around in his lab, I felt at home immediately. I later visited him several times, and he introduced me to many of his friends in the wonderful NIR community.

Karl and I never discussed politics and religion, - we would probably have disagreed about some things, for we came from different cultures. But I think we shared a common view of how to understand the physical world and about how we as researchers ought to use our time here. We clearly agreed about the importance of measuring real-world qualities in real-world samples to solve real-world problems. Gradually, I learnt to see the value of math, statistics, computers and programming, and of having the human in the loop when combining our prior knowledge and our modern measurements.

Karl showed me his interactive version of "machine learning" - how he developed calibration models for getting value out of per se meaningless NIR spectra from his scanning CARY instrument. Mathematically, his system was based on multiple regression on statistical combinations of sums and ratios of measurements at different wavelength channels. Statistically, it was very parsimonious and thus easy to validate. But it was also graphic and highly interactive, - it allowed him to use his human background knowledge. Different from anything I had seen in statistical software, including my own!

Using spectral derivatives in chosen wavelength regions, his interactive regression plots revealed and quantified *additive* absorbance variation patterns - allowing him to correct for the unwanted variations, known or unknown. OK, through the '70s I had also discovered some of that, working long nights alone at the University's main computer to make psychometric PCA and MLR useful for chemists. But by interactively *ratioing* pairs of spectral derivatives, he also removed unwanted, *multiplicative* path length effects in the same process! On top of that, he interactively eliminated wavelength regions that he did not find useful. I returned home, surprised, confused and deeply impressed. T*he MSC was just an attempt to copy Karl*

At the Norwegian Food Research Institute we got our first NIR reflectance instrument (Infralyzer 400) in 1981. The instrument had only 19 fixed wavelength filters, but it was easy to use, and gave very, very precise reflectance data R. One day, after I had tried - in vain- to mimic Karl's spectral derivative ratioing for our fixed-filter instrument, I plotted each food sample's "19-channel absorbance spectrum" on the y-axis against their average "absorbance spectrum" on the x-axis. Immediately, a statistical equivalent of Karl's derivative ratioing became obvious: The different samples' spectra formed different, almost straight lines. *Subtracting* for the line offsets mimicked Karl's spectral *derivatives* and, at the same time, *dividing* by the line slopes, mimicked his multiplicative spectral derivative *ratioing*. I named the method "Multiplicative Scatter Correction, MSC". Later, after we saw that the same preprocessing was also applicable to chromatographic profiles and taste panel evaluation data, I started to call it "Multiplicative Signal Correction".

In the future I believe we shall see a merger of modelling principles from the MSC-type preprocessing and PCA/PLSR-type subspace data modelling, in a dynamic feedback setting of control theory. I am still surprised at how useful is mathematics. But for me personally, it has all been strongly based on Karl's warm inspiration and courageous ideas, and on my jealousy of his Cary scanning spectrophotometer.
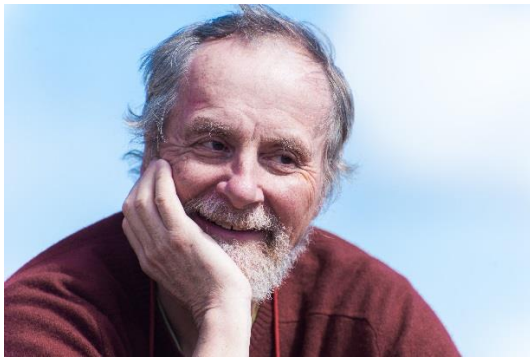
Harald

Contribution from Yukohiro Ozaki

Karl, his wife, Fred, and me at EAS in 2001. I received the EAS award for NIR spectroscopy. Karl and Fred encouraged me a lot and we had a very nice time together.
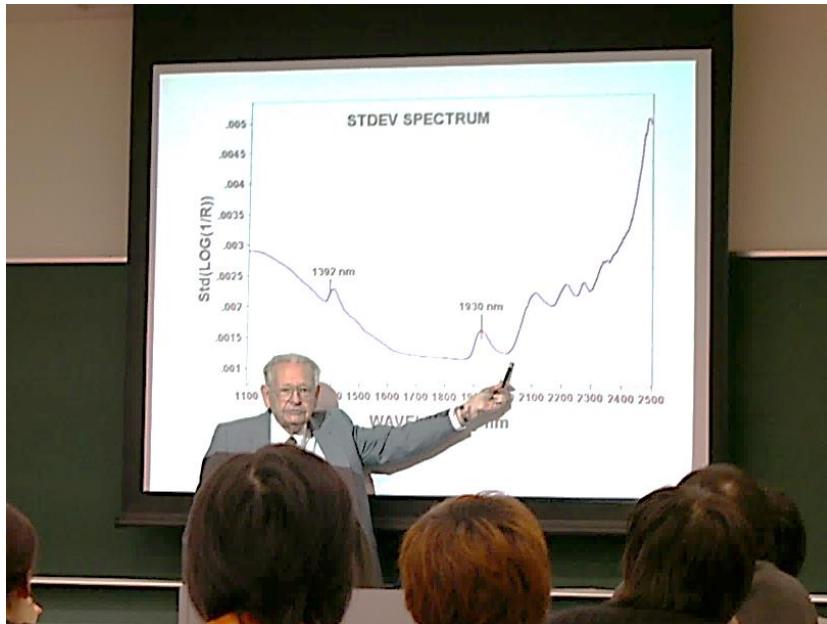

Karl with Maxine at EAS in 2001

Fred and me at EAS in 2001

Karl kindly gave a lecture at School of Science and Technology. Kwansei Gakuin University. He talked about the history, basic principles, characteristics, and applications of NIR spectroscopy. We were all very much moved by his enthusiastic lecture. After this lecture we went to a Japanese restaurant nearby to have a wonderful dinner together.
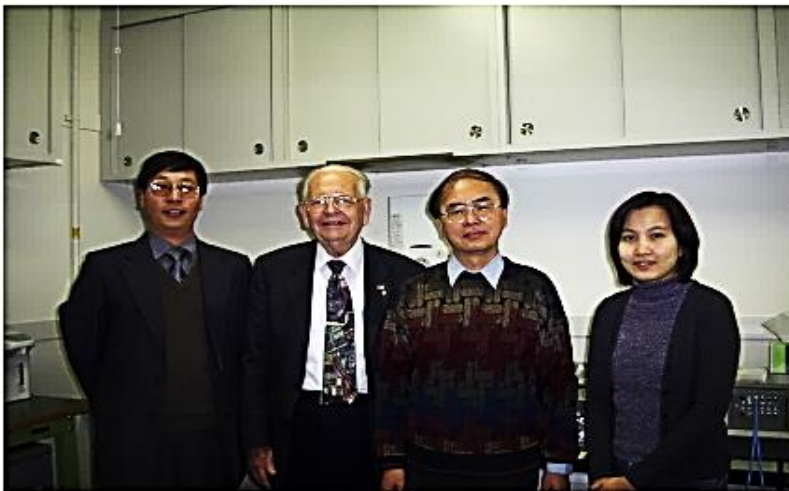
Karl at my lab in 2003. From left to right, Prof. Yiping Du, Karl, me, and Dr. Sumaporn Kasemsumran. Karl looked around my lab. and enjoyed very much discussing with young people. He was also an excellent educator.

Karl was always a gentle father. He did encourage young people. He had a number of children in research, grand children, and great-grand-children, all over the world.

Contribution by Gary Ritchie

A Quick Note on Karl Norris

This summary is from work that Karl brought to my attention. He had asked me if I would collaborate with him on writing up some experiments on the Chambersburg Shoot-out 2002 data set (On Calibration Transfer) (Journal of Pharmaceutical and Biomedical Analysis 48 (2008) 1037–1041. In his own words, Karl discuss's what utility he saw in the data set that Emil Ciurczak developed and that I produced with a young and enthusiastic team of scientists at the Purdue Pharma Global Research Center in Ardsley, NY. Karl was gracious in acknowledging our contribution to his work. This was characteristic of him. He expressed his hope that I would agree to help him, mostly in explaining the regulatory implication of specificity as it is applied to pharmaceutical tablets, but also some nuances of the data set. I accepted. While this work brought me closer to Karl the scientist, what I really enjoyed most about Karl were the few times I got to visit with him at the Chambersburg Conferences and several other meetings where he presented and where he exhibited his sense of wit, humor and his coolness.

Not only has the 2002 Chambersburg data set made it around the world multiple times as a teaching and diagnostic tool since its development, but Karl saw its potential for use on demonstrating an idea he was developing based on some of his observations on NIR specificity. He theorized that specificity could be demonstrated by showing that if the first principal component spectrum is shown to match the spectrum of the Active Pharmaceutical Ingredient (API), difference (high assay - low assay) and averaged spectra from two MultiTab transmission instruments extracted from the original data set files; the criteria for specificity could be met. In fact, he believed the new criteria demonstrated from this novel approach could serve as a Figure of Merit establishing causality of the correlation (r) regression and bias based solely on the API and not analogs or API degradants.

He theorized that the Chambersburg data set was optimal for testing a hypothesis for specificity of NIR spectra because of:

1. The many samples (thus spectra), measured on two instruments,
2. The API has relatively narrow absorption bands (covering both short and long wavelengths) and
3. The instrument noise is low enough to permit little smoothing.

These features were significant to Karl because they lent themselves to applying several tools he had in his tool box and honed over his career for developing strategies for analysing NIR spectra: API extraction, spectral subtraction and derivatization.

Karl revealed several properties of NIR specificity based on his observations with this data set. Because he showed that it is possible to extract spectra from the data set that matched the spectrum of the API, he postulated that:

1. Since spectra were used from two instruments, spectra from both instruments were included in the high and low value sets, and averaging the spectra reduced the effect of instrument noise to provide a better match to that of the API spectrum.

2. By using this second-derivative conversion, regions of the extracted and API spectrum show enhanced absorption features, producing negative peaks that can then be used for comparison at the wavelengths of the absorption bands to more clearly show the degree of match. The positions of the negative peaks are the best evidence that the spectra match.

3. The spectra of the first principal component, the API, and the extracted spectrum should match very well after converting each to the second-derivative format.

Based on these observations following the comparison, Karl took the necessary leap and made a bold proclamation: all [15 of the] negative peaks of the API and the extracted spectrum match on the wavelength scale within 1 data point to that of the first principal component (PC 1). This provides assurance that a calibration is specific for the API.

But Karl did not stop there. He challenged his own conclusion by performing other pre-treatments combined with outlier removal, and in separate experiments, adding noise to the extracted spectral data set to demonstrate the robustness of this method for determining specificity. Only after further meticulous experimentation does Karl relax and comment that the utility of this procedure for NIR specificity differs from other tests proposed for specificity that depend on the use of active substances or excipients close to the API tested and forced degraded samples. Instead, he proposes the novel use of the high–low extracted spectra and compares their differences to the first principal component spectrum of the model and the pure API spectrum for verifying specificity of the calibration model, and for showing the suitability of its intended use for assaying API concentration. In other words, to paraphrase Karl, the correlation (r) regression and bias of a NIR calibration model may be shown to be due to the range, signal to noise and absorption properties of the API spectrum solely and need not to be shown using analogs of the API as surrogates for specificity.

In this one exercise, we get to peek inside the meticulous mind that Karl possessed by following his observations, his line of inquiry by experimentation and to also being touched by his bold and courageous heart. I am also sure that all of us who got to know and work with him came away with the same sense of awe, adventure and pure joy that Karl did in playing with Near Infrared spectra.

IDRC 2006 (The Chambersburg Meeting 25th Anniversary)

CNIRS members join IDRC Chairman Gary Ritchie and Dr. Karl Norris (Hon.) to cut the commemorative cake celebrating 20 years of the CNIRS and 25 years of the IDRC. Front: Gary Ritchie, Karl Norris, Back: Carl Anderson (President, CNIRS). Fred McClure, Dave Wetzel, John S. Shenk, Franklin Barton, Howard Mark, Tony Davies and Phil Williams.

Contribution by Dave Ryan

Fond Memories of the Master of Masters – Karl Norris

David J. Ryan, Principle Scientist – DuPont Nutrition & Biosciences

It is with significant sadness that IDRC 2020 has been canceled. This meeting has always been a highlight of my career, and doubly so as we will not again in this lifetime be graced to listen to the Master of Masters, Karl Norris, address the conference attendees at Wilson College Science auditorium and impart his wisdom. His presentations and understanding of the subject matter rose above the insights of most, and always provided unique perspectives that no one else had. His interpretations of the IDRC Shoot Out Data was second to none. His presentation of the Shootout dataset was always last, like one might experience at Christmas time, by saving the best gifts to open at the end.

I am profoundly grateful to be involved with NIR and Diffuse Reflection at a time of exponential growth in the field that generated tremendous excitement and career opportunities. There are only a few individuals that have impacted my career so profoundly. One is John Shenk and the other is Karl Norris. I can humbly say that any success I may have achieved over the years is no small part to being able to stand on the shoulders of giants. Apart from the excellence in science and engineering, and even more important, was his humility and friendliness to all. He took the time to spend with you to address any questions that you may have. I considered him a personal friend, but all one had to do to achieve this status was to meet him and talk to him once. He would always greet you with a smile on his face. Even in later years his passion and drive were simply amazing.

His interpretation of NIR spectra was second to none. I can only imagine how many hours he must have spent studying and learning NIR spectral bands. 2nd derivatives were his preferred math treatment. While others relied on more sophisticated chemometrics, he relied on visual analysis. Increasing concentrations were in in the negative direction for Log I/R NIR Absorbance spectra and allowed band assignments to match literature assignments. His favorite algorithm was his touted 2nd derivative ratio division math algorithm followed by MLR.

$$\frac{d[f(x)]}{dx} = \frac{f(x+gap) - f(x-gap)}{Norm}$$

He would find spectral nodes near the constituent band of interest that did not change. This would represent the denominator. The band that represented the signal would be in the numerator. The second derivative involved a gap, with smoothing. All this had to be optimized from many iterations. The last version has been coded in Matlab on which David Hopkins and Karl collaborated. This is open source code available to anyone who is brave enough to learn. This has been well documented by David Hopkins, *Vol. 27, No.7, October 2016, <u>NIR News.</u>* My only attempt at using this was from early versions found in NSAS. I learned quickly that to fully take advantage of its capability took some mastery that I did not have the time to develop. His latest efforts focused on the interpretation and modeling using 4th derivatives, which to my knowledge no one has successfully implemented in any robust applications.

He was also a master at understanding the physics of light and instrument design stemming from his electronics background, which was also put to good use by him while serving our county in

World War II. He understood weaknesses in instrument design, and as a result, avoided regions of the spectra that would add noise, anomalies, and non-linearities. Using all of his understanding, he was at times able to create models that had the robustness to be able predict accurately beyond the modeling range. During one NIR meeting we were having a conversation around a published article that described a number of sophisticated chemometric approaches. He had access to the dataset and using his magic was able to obtain correlations better than was documented in the publication, but his humility never allowed him to tout this in a public way.

Personally, I sought his expertise on a problem I had in working with the Foss Beverage analyzer. This unit operated in transmission with a fixed pathlength for a single application but was adjustable for different applications. Fiber optic reflectors were located inside round quartz tubes. Not your typical square fixed pathlength cuvette. As a result, he helped me understand that the spectra produced was a combination of a variety of pathlengths, smallest at the shortest distance and longer at the edges.
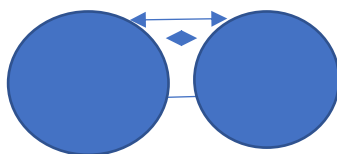
Being there is an optimum pathlength to maximize S/N, and minimize non-linearity, the spectra, by definition, were always a blend of ideal, and non-ideal, therefore contained significant non-linearities. Especially samples with different opacities, which we had to deal with, created a whole new set of pathlengths and problems. His advice provided the insight necessary which helped me make the calibration as good as possible, given the limitations. There will never be another Karl Norris. He was the best person at the right time to advance the science. Without a Karl Norris or a John Shenk, I venture to say I would, and maybe many others, would not be putting this technique to practical day to day use.

I would like to thank Phil Williams for giving me the opportunity to say a few words to the IDRC community and best wishes to all. I hope that IDRC 2022 once again is able to bring our IDRC family back together. The picture below is from IDRC 2000, when we were all much younger. I am on the left. I believe David Massey is on the right.

Thanks.

David J. Ryan.

Contribution by Mui Saranwong

The NIR Grandfather

My memories of Karl are a bit different. They are more personal than about NIR. I first came to Japan to learn NIR in Oct 2000. When my Professor, Sumio Kawano, picked me up and drove me to Tsukuba, he told me "You are a lucky person, you will have a chance to meet both Karl Norris and Phil Williams in the same trip." Later in November of that year, the Japanese NIR group invited Karl to Japan. I was as afraid of him as any Thai girl would be in fear of meeting the great scientist. I found that he was very kind but very quiet. I, who knew nothing about NIR, felt very impressed by his warm smile. An unforgettable memory was when we went to a tempura restaurant in Tsukuba. The restaurant was very old and nothing that would appear to be fit to welcome "The Father of NIR spectroscopy" but yet he never complained. We signed the restaurant book together, and had a very good and tasty tempura dinner.

A few years later, the Japanese team established the Karl Norris (FANTEC) Award. We invited Karl to become the first winner. That year, we had Karl and Graeme Batten as our guests. Karl said he wanted to buy pearls for his wife, Maxine. He was unhappy with the choice in Tsukuba because they were not Japanese pearls. Later in the week, we went to the Mikimoto shop (the shop that makes Miss Universe's tiara) and we found something that suited Karl. I will never forget the warm smile of Karl's satisfaction.

On another occasion (I cannot remember which year it was); we were at the MacDonald's near Mt. Tsukuba together with Sumio and his son. Sumio said "here we are, 4 generations of people". For me, Karl is as sweet as any Grandpa could be. We had a great talk one day when he found out that I was a biologist. He told me that his greatest invention was actually being a major part of the discovery of Phytochrome.

I will not say I am sad or sorry that he is gone. I think he had lived his life. In his own time he was, and still is The Legend, and I would never become who I am now without his innovation.

Thank you, Karl! I know you are up there and smiling as always.

Mui Saranwong

Thailand
Secretary of the ICNIRS

From Left to Right, FANTEC staff, Karl, Mui, Miho Fukami and Mikkabi staff. Taken at Mikkabi satsuma mandarin sweet sorting facility, Shizuoka, Japan 2000.

Contribution from Russ Tkachuk

A tribute to a Great Scientist

It is a privilege to write a tribute to Karl H. Norris (23 May 1921 - 17 July 2019). Karl's report that NIR should be very useful for grain analysis in 1965 seemed like a very useful concept, especially for a grain producing country like Canada. So, near infrared reflectance (NIR) studies began at the Grain Research Laboratory in 1972. The application of NIRS to on-the-spot determination of protein content of CWRS wheat was originally in reflectance mode on ground wheat, but in 1990, following the introduction of the Infratec by Tecator of Sweden, this gave way to whole wheat in transmittance mode, the method in use to date. The test is complete in less than a minute, and requires no laboratory experience for its execution.

I visited Karl in his Beltsville laboratory and met him numerous times at various scientific conferences. He was very interested in my work with Don Law on the chemistry of NIRS, and particularly on our identification of the main wavelengths of wheat components. He was always very generous, in giving useful suggestions and advice to NIR queries, which was always given in

a willing and friendly manner. So, Karl Norris, "Rest in Peace", and "Thank You" so very much for all your help and useful advice.

Russell Tkachuk, Sechelt, B.C. Canada.

Contribution from Roumiana Tsenkova

Water and Light
In memory of Karl Norris, Kobe, May 16, 2020

For all of us, the NIR community, Karl was like water and light. We felt comfortable in his presence, relaxed and with great respect. We learned a lot from him and his attitude taught us to be like him. His questions and comments were the light into the invisible NIR light that led us towards opening new venues and unexplored worlds.

My gratitude to him is beyond any description! In my memory, there is a moment which I will always remember. At the NIRS International Conference held in Korea in 2001, for the first time, I presented something that caught my attention when analyzing real time spectral data of prion proteins isomers and I wanted to check if the phenomenon has been caused by water. At the conference I presented my results that the water spectra change after each measurement, and showed that these small changes in absorbance (stable microscopic changes of absorbance) have information about the number of the measurements, the time and the solvent. After the talk, Karl came to me and said: "Very well done! If you subtract the spectrum of water from the spectrum of protein solution, you will never see the spectrum of protein. Water is interesting." This gave me the courage to continue working in this direction and to introduce Aquaphotomics and name it as a new -omics discipline at the International NIR Conference in New Zealand in 2005. Since than Aquaphotomics has grown and this year we planned our 4th International Conference on Aquaphotomics to be held in Kobe, Japan.

Karl was not only an engineer; he was full of curiosity, a constant learner and a discoverer. We were all so pleased when he was awarded the honorable doctor degree from Wilson College (see picture from the ceremony). He really deserved it! And he was really happy to receive it!

Karl and his wife Maxine were very kind and friendly. They have invited me to stay with them when I attended Chambersburg meetings. I have been touched by the fact that "the great Karl Norris" would come to pick me up from the airport whenever I visited them and especially at his age in the last years. We have had numerous conversations about everything: life, science, friendship.

Karl Norris will be always the LIGHT among us, in our memories and hearts!

Peace be with you!

Prof. Roumiana Tsenkova, Dr. Eng., Dr. Agr.

Kobe University,

Biomeasurement Technology Lab

With Karl Norris and Karoly Kafka, two pioneers.

Karl Norris awarded with honorable Doctor of Science degree from Wilson College

Karl presenting Prof. Ozaki's talk at the Gerald Birth Award Ceremony at IDRC-2006

Contribution by Lois Weyer

The first time I met Karl was when he and I were standing in line to register at a hotel, probably in Chambersburg on a weekend before one of the early symposia. I was awe-struck at meeting the person who started the whole field of modern NIR and he was very kind and friendly. He continued to be helpful and welcoming to me, as a newcomer. And, we proceeded to see derivatives in the same way throughout the following years.

Lois

Contribution by Phil Williams

My memories of Karl

My memories of Karl stem partly from the many conferences that we have both attended, and partly from the memorable year November 1976-Novenber 1977, when I was privileged to work with him in his laboratory in Beltsville, MD.

The conferences included the IDRC conferences, held every even year at Wilson College, Chambersburg PA, and the international conferences, which rotated among countries each odd year. During the second IDRC conference in 1984, Karl and I sat with Gerry Birth, the founder of the IDRC conferences, and discussed the concept of a monograph that would assemble every aspect of NIRS. The monograph was duly assembled, with contributions by experts in all of the aspects. At all of those conferences, beyond greetings, I purposely stayed away from him. He was

continuously surrounded by NIRS workers, young and seasoned, who sought his knowledge, and advice, and who only had the opportunity to share his wisdom on those annual occasions. So my memories of him at conferences were mostly of him in a head-to-head huddle with someone, or with a small cluster of acolytes.

An excellent example of his benevolence occurred during the memorable 1986 conference in Hungary, when the ICNIRS was founded. One afternoon there was a sight-seeing bus-trip. On the way out I was sitting beside a young lady, who asked me questions about application of NIRS to determine apple quality. After we had discussed the things that she could do (including identifying the factors that affect the variance in apples, and assembling sample sets), she mentioned that she would like to have met Mr. Norris. At the first stop I introduced her to Karl, and told him that she would like to ask him some questions, She was with him for the rest of the trip, and I'm sure that she has the same sort of memories of him that I and many others have experienced.

He and I carried out our conversations by telephone, whenever the occasion demanded, usually whenever I needed to know something about the spectroscopy. Our conversations were short, because he always had the answers, and both of us were busy. I had the privilege of working with him for a full year in his lab in Beltsville MD. During the first 1 or 2 days we talked about the evaluation of calibrations. He showed me his results on prediction of the protein content of wheat, using his second derivative quotient math algorithm. He had combined 6 sets of wheat samples, and had obtained a SEP of 0.066, after 8 iterations. I asked him what would happen if he calibrated on 5 sets and predicted he other one. He said that the result would be the same, so I asked him if we could try it anyway and we obtained a SEP of 0.27. He was a bit surprised at that, but I said that that was probably the right result. Then we returned the predicted sample set to the combined calibration set and repeated the procedure, using another set, and this time the SEP was 0.26. I pointed out that to evaluate a calibration it was necessary to predict a set that had not been used in the calibration of which, to my surprise he had not been aware. He arranged for the head statistician of the USDA to come to talk with us, and he, of course said that that was indeed the true method for evaluation of a calibration. In other words, Karl had been using the SEC all along, up to then. So Karl actually learned something from me, but I would like you all to know that he learned something from all of you who were privileged to talk with him. You all contributed to his wealth of knowledge.

During our year together we addressed the variables of particle size and moisture content in predicting protein content of ground wheat. I designed the experimental work, and arranged for all of the samples to be assembled, and sent from the GRL, Winnipeg, including all of the laboratory analysis. My colleague, Dr. Susan Stevenson, did a great job on assembling the sample sets for us. I set forth to do the calibration work, using Karl's Cary 14 spectrometer and his quotient math software. The first thing that I learned from Karl was how to access his computer and its software. I got my ball-point pen and a note-pad, and took notes from Karl. When I was through, I had 12 pages of notes on which switch to toggle and in what sequence, and what the screen should say. It took about 3 minutes to get his system running. From time to time in the early days I would make a suggestion about a small change that would make things a bit easier. Next morning, I would be chagrined, to find that I couldn't get the computer up. He would emerge with a sly smile, explaining that he had made the change that evening and changed the toggling process! Eight months later in August, when the calibrations were all complete, we sat down to see what we had

achieved with his quotient math algorithm. After testing 6 or 7 calibrations, and used them successfully to predict protein content in samples that differed very widely in particle size or moisture content, using reciprocal calibrations, Karl quietly said "I think we have a breakthrough". That moment will stay with me forever.

Later that year (1977) we introduced these applications of his quotient math pre-treatment at the AACC annual conference in San Francisco. I was spellbound by the diversity of his vast knowledge of spectroscopy, from the ultraviolet to the near-infrared, as well as his knowledge of the voluminous aspects of operation of the equipment, all of which he enjoyed to share freely with anyone who sought his expertise. But there is more in life than NIRS, and during the year I learned about Karl Norris, the Man, his subtle sense of humour, that would emerge unsuspectingly from time-to-time. Also his fondness for his monthly poker evenings with some of his colleagues, to which I was invited. His remarkable memory often came to his aid during those evenings, to the frustration of the rest of us!

Truly a memorable year, and the founding of a collaboration and friendship that persisted for 44 years. After his retirement I called him every few weeks, and our conversations were a lot longer than during his working days. He grew very sad when he began to lose his memory, and could no longer use his software. We continued to enjoy our telephone conversations until only a few days before he left us, on July 17th, 2019, and bless him, he remembered my voice right up to the end.

From Phil Williams
August 6th, 2019.

Karl and me at an IDRC

Contribution by Jerry Workman

In talking with Karl, I recall that he was always interested in interactively discussing any problem or issue associated with NIR. He really came alive when any problem or challenge was presented

- either one-on-one, or a small group, or an auditorium full of scientists - when a problem was introduced, Karl was all in! And he usually had experienced something similar or would propose a solution that was scientifically sound and would eventually turn out to be the answer. He always was enthusiastic, friendly, and exhibited a kind smile no matter when and where you ran into him. When they say the phrase, "a scholar and gentleman," that characterizes Karl magnificently! He will be greatly missed.

Jerry Workman