SAS SPECTRUM eNEWS

Student Ambassador Report for the 14th Annual Chemometrics in Analytical Chemistry Conference

Contributed by Brett Brownfield

The 14th Chemometrics in Analytical Chemistry conference was held in Richmond, Virginia, from June 9–13, 2014. Thanks to the student ambassador award provided by the SAS, I presented a poster at this conference entitled "Improving Outlier Detection by Fusion of Outlier Detection Merits Using Sum of Ranking Differences", and was awarded a first place prize.

The content of the conference included a broad range of spectroscopic topics including "-omic" applications, imaging, and computational modeling. There were a total of nine plenary and keynote lectures, 40 oral presentations, and 70 posters (which were on display for the entire conference). Even though the conference was held in the United States, there were 142 participants from 26 different countries. Thankfully, the schedule had built-in coffee and lunch breaks that encouraged networking and conversation. The conference also hosted off-site excursions, which enabled me to visit the Science Museum of Virginia and attend a banquet at the Virginia Museum of Fine Arts.

All these events provided opportunities throughout the week to promote the benefits of joining SAS among the younger scientists. I placed emphasis on the numerous student programs and opportunities suited for career advancement, in particular the new Bruce R. Kowalski Award. I also talked about Applied Spectroscopy and explained that online versions of the journal are free for SAS members. I really enjoyed being an ambassador, as it encouraged me to converse with more people than I would have otherwise. I had a great time and hope to see the SAS membership grow.

Brett Brownfield is a PhD student in the Kalivas Group at Idaho State University

Brett in front *of* a Thomas Jefferson statue.

Outside of the conference venue, the Jefferson Hotel.

Near-Infrared Spectroscopy in China

Contributed by Heinz W. Siesler

Introduction

On the occasion of the recent EuroPACT 2014 conference in Barcelona (May 6-9, 2014) and during a lecture tour to China (June 5-18, 2014) I met numerous Chinese scientists who practice in the field of near-infrared spectroscopy. In this short report I would like to summarize these impressions, which are further supported by cooperation with a guest professor (Prof. Dr. Xiong Zhixin, Nanjing Forestry University) who presently spends a one-year sabbatical in my research group.

My visits to two Chinese universities were actually initiated and partly organized by a Chinese industrial scientist (Prof. Dr. Wei Hansen) who lives in the Netherlands after her retirement from Unichema International. Her company and invaluable assistance before and during part of the trip was the basis for the successful mutual transfer of expertise between me and the research groups of the visited universities.

After getting a first insight into the important role of near-infrared spectroscopy for process analytical technology in a multiplicity of Chinese industries such as the food, pharmaceutical, refinery, and chemistry sectors from the plenary lecture on "Process Analytical Technology and its Future in China" by the present chairman of the Chinese NIR Council, Prof. Dr. Hongfu Yuan (Beijing University of Chemical Technology) at the EuroPACT 2014 conference, I had the chance to compare the presented data with actual activities in this research field during my subsequent visit of the School of Biotechnology, Jiangsu University, Zhen Jiang, and the Information Engineering Center at Ocean University of China, Qingdao.

Visit to Jiangsu University, Zhen Jiang, Jiangsu Province

Prior to my lecture on recent developments and applications of near-infrared spectroscopy I was appointed as guest professor to this university. The rest of my visit was dedicated to the discussion of research topics of mutual interest with members of the School of Food and Bioengineering. Prof. Dr. Bin Chen, the Head of this department, who is very successful in the acquisition of industrial projects, had gathered not only his present, but also several previous coworkers and graduate students for a very intense and productive discussion. The research focus of his group is instrumental as well as application oriented. Thus, a state-of-the-art interface by which an application (app) runs on a smart phone to drive a handheld spectrometer (JDSU, MicroNIR 1700) has been recently developed. Based on this system NIR spectroscopic data are taken on-site on fruits and herbs (for traditional Chinese medicines (TCM's)) to develop calibrations for the determination of relevant food parameters or the geographic origin. Discussion contributions of former coworkers demonstrated that many of them work in spectroscopy-related jobs where they could implement the expertise gained during their previous university education. Most of the described projects can certainly be ranked up front on an international level of near-infrared spectroscopic research. Apart from scientific problems, we also addressed topics of general interest such as the role of women in science and Chinese society. I was specifically impressed by the relaxed human relations between the supervisor and his present and former coworkers, and thoroughly enjoyed the open discussion on the multiplicity of topics. In summary, it was a typical situation where a healthy climate of communication creates an environment for productive and successful research.

Visit to the Ocean University of China, Qingdao

My final days in China were dedicated to a visit to the Information Engineering Center at Ocean University of China, Qingdao. The team of this department is headed by Dr. Yang Ning, who performs research in near-infrared spectroscopy on a broad range of topics. The changes from benchtop spectrometers to handheld systems for more flexible in-the-field measurements including the calibration transfer from the laboratory to the

miniaturized systems are relevant issues. My lecture on novel developments and applications of handheld spectrometers therefore fitted perfectly in their research interests. Most of the time we spent discussing the ongoing research project on the impact of geographical origin of tobacco leaves on the content of toxic components and related health risks which is certainly not only a topic of relevance to the Chinese society. Specifically, we discussed the strategies of calibration development for selected parameters based on the near-infrared spectra measured in diffuse reflection of dried and milled tobacco leaves. Here too, the research work in this department is driven by interdisciplinary cooperation, dedication and persistence.

Personal Conclusions and Comments

The two research groups I was able to meet during my visit to China perform state-of-the-art research in near-infrared spectroscopy and are competitive to other international research institutions. Any of my discussion partners could be easily integrated as a coworker in a US or European research project in this field. I have to admit, however, that the smooth communication during my visit would not have been possible without the dedicated interpretive assistance of Dr. Wei Hansen. Being a spectroscopist herself, she perfectly managed to transfer mutual ideas and contributions to make the discussions fluent even in situations of complicated topics.

China has a huge potential of talents in the field of spectroscopy and I can only encourage SAS to:

(1) Strengthen the ties to China, for example by sending delegates to conferences in China
(2) Encourage young Chinese scientists to join research groups of SAS members.
(3) Improve the mutual scientific exchange for the benefit of both sides.

Regarding the general technological developments in China since my last visit in 2010, my impressions are ambivalent. On the one hand, China has made substantial progress in the development of public transport to a point where it has overtaken the US and partly Europe, and is close to catching up with Japan. But on the other hand it has neglected the problem of air pollution to a point where it puts the health of its population at stake. During 12 of 14 days of my stay in China a dense layer of smog darkened the sky not only in the cities, but also in the countryside. Only during the last two days in Qingdao, a popular seaside resort in China, blue sky came to the fore. Let us hope that the political authorities recognize this ecological problem and take urgent action before it is too late.

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Section News

Prof. Tim Keiderling is presenting "Protein Folding Starting From the Ground Up: Thermodynamic and Kinetic Spectroscopic Studies of Peptides and Proteins With Increasing Complexity." at Saint Anselm College on September 17, 2014.

Contact Ellen Miseo, ellen.miseo@gmail.com, for the full announcement. Phone: 413.366.1491

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