SAS SPECTRUM eNEWS

Editor's Note

Richard Crocombe graciously accepted our invitation to write a short commentary on portable spectroscopy for this issue. The topic of portable spectroscopy is very dear to my heart and I am not exaggerating to say that my career was changed by it. When I started my current role as an analytical scientist in 2008, most of the analyses were carried out based on samples brought to our labs; benchtop instruments were used to perform the analyses. While the process analytical field was already a well-established discipline back then, it was often meant for permanently installed process analyzers and rarely for the troubleshooting of one-off process upsets or problem solving. When a project need arose that required us to deploy a probe into a lab reactor, we had to scramble to borrow various components so that we could bring a spectrometer to our collaborators' synthesis lab. The success and otherwise inaccessible information enabled by in situ spectroscopy really changed my career as we then became able to justify the acquisition of multiple portable spectrometers. Now, more than half of my work leverages our now well-established portable spectroscopy capabilities to various business groups and sites within my company. I even once travelled internationally, carrying a ReactIR, a B&W Tek Raman, and a MicroNIR system literally with me onto the plane. Such a feat would not have been possible without the tremendous progress made in the field of portable spectroscopy. I hope that the readers will find Richard's piece informative and helpful for defining further opportunities to apply spectroscopy to an even broader application field and to address more problems.

Contributed by Shawn (Xiaoyun) Chen
xchen4@dow.com

Join Us for the Following Special Events at our SAS National Meeting During SciX in Atlanta

Sunday, October 21 – 7:00pm	**SAS Student Poster Competition* and SciX Opening Mixer** Marriott Marquis
Monday, October 22– t 8:00pm	**SAS Student Members Only Event*** Braves All Star Grill, Downtown Atlanta

Tuesday, October 23	**Special 60th Anniversary Sessions** Marriott Marquis *Past, Present and Future: Celebrating 60 Years of SAS and Spectroscopy Innovations*
Tuesday, October 23 – 7:00pm	**SAS Awards Ceremony** Marriott Marquis Imperial A
Tuesday, October 23 – 8:00pm	**SAS 60th Anniversary Wine and Cheese Celebration with Special Entertainment** Marriott Marquis Imperial B This event is open to SAS members only* from 8:00-9:30pm. A group SAS commemorative photo will be taken at 8:30pm. Doors will open at 9:30pm to non-members.

*Not an SAS Member, but want to be part of our Member's Only Events?
Join SAS today and be part of the next 60 years!
Visit www.s-a-s.org or call 301-694-8122 to join today!

New York SAS Section Announces the Forthcoming Meetings

The New York/New Jersey section of the Society for Applied Spectroscopy is pleased to announce the new meeting schedule coinciding with the next academic year, beginning in September 2018. The following speakers will be presenting their work, as well as others for future meetings:

September 13, 2018: John Wasylyk, "Application of FTIR in Understanding the Changes in Protein Secondary Structure as a Result of Stress" (tentative title) to be held at Horiba Scientific, 20 Knightsbridge Road, 08854, Piscataway, New Jersey.

October 2018: Christine Sayhoun, title: "A Comparison of Structural and Functional Optical Coherence Tomography Systems for Assessment of Hard Dental Tissues"

November 2018: EAS Gold Medal Award Program honoring Professor Igor Lednev, University of Albany sponsored by NY/NJ SAS and EAS, held in conjunction with the Eastern Analytical Symposium (EAS).

December 5, 2018: Curtis Marcott, PhD, Special Tour Speaker meeting, title to be announced.

Due to the required lead times for publication, we have to make this announcement before we have all the details of the meetings arranged. Everyone interested in attending a meeting will find the meeting details posted on the NYSAS website at www.nysas.org as soon as they become available. Please consult the website regularly for updates about the meeting details, as well as possible changes and information about future meetings. If you plan to attend a meeting, please email the NY/NJ SAS secretary, debperu@outlook.com, beforehand so we can make arrangements for the expected number of people. Your name will also then be added to our email list for future meeting announcements, unless you request to not be added.

Contributed by Howard Mark
hlmark@nearinfrared.com

Portable Spectroscopy

The Society for Applied Spectroscopy (SAS) and the journal, as their titles imply, are the home of applied spectroscopy for the academic and industrial spectroscopy community. Clearly, those practitioners in specific areas (e.g., biomedical spectroscopy) are members of other communities, and will be up-to-date with the literature in those areas. First, portable and handheld spectrometers are related to at least three other fields. These include very practical applications in specific areas like hazardous material identification, pharmaceutical QA/QC, law enforcement and street narcotics, etc., which will have their own journals and magazines. Second, the technologies employed in small and miniature instruments may come from research institutes, government laboratories and small companies doing government-sponsored R&D (e.g., Small Business Innovation Research [SBIR] funding), and presented at SPIE meetings. (Luisa Profeta described SAS member involvement in an SPIE conference in the June 2018 newsletter.) Third, there is an emerging area of miniature spectrometers marketed directly to consumers, and the companies involved may exhibit at consumer electronics shows, for instance, CES in Las Vegas (https://www.ces.tech/), and not at scientific meetings.

As applied spectroscopists, trained and familiar with issues like sampling, spectroscopic databases, algorithms, calibration and validation, etc., we should be aware of and engaged with organizations doing miniature spectrometer development, and those producing instruments sold directly to consumers. There is certainly an "educational" goal here, and that involves outreach to non-SAS (non-SciX, non-Coblentz) organizations and publications. So I'd challenge SAS members to promote spectroscopy by engaging in discussions on these instruments and offering advice to people and emerging companies who have technologies, but are not grounded in analytical spectroscopy, and could therefore make false assumptions or unrealistic application projections.

As an example, last year Ellen Miseo (former SAS President) and I wrote an article for Photonics Spectra on spectroscopy for food fraud detection. We focused on two major areas in which claims have been made for the capabilities of handheld optical instruments: heterogeneity and detection limits. We made the case that these are poorly understood areas in the "consumer spectroscopy" arena, and that both the companies involved and the potential customers need to understand this. As a practical example, we used blueberry muffins as an example of heterogeneity and surface versus bulk composition. (A very similar heterogeneity issue exists for mineral characterization using handheld XRF [or handheld LIBS].) Handheld XRF will interrogate a spot size of about 1 mm to 8 mm diameter, and LIBS instruments use a much smaller spot, but can raster the beam. However, to obtain a reliable picture of the average composition of a mineral, the standard practice has been to grind the sample and press it into a pellet for analysis, as opposed to doing single spot analysis.

How do you run the optical spectrum of a highly heterogeneous sample with a portable device, and what reliable or comprehensive information will you obtain? (Photo by Eric Crocombe)

Recently, I gave a webinar for Photonics Spectra on portable spectroscopy. This covered the fundamental technologies available, and how they are used in both complete devices and the "engines" available to be built up into products. One section described how the traditional companies in this area have placed a lot of emphasis on building their own quality-controlled databases, and using algorithms appropriate to the specific task to give the non-scientist user immediate, confident, and actionable information. This is in contrast to some of the direct-to-consumer companies, employing crowdsourcing of data, and generation of "answers" in the cloud, using non-disclosed algorithms. The lack of quality control for the incoming "database" or "calibration" data has to be a major concern for an analytical spectroscopist.

Briefly, the webinar also covers areas like the rationale and value proposition for portable spectrometers, their use cases and "ideal" (point-and-shoot) characteristics, market drivers, overall background and history, overview of existing instruments, size and shape of portable instruments ("cordless drill" and "paperback book" form factors), new miniature spectrometer "engines", the development of "smartphone" spectrometers especially for clinical diagnostics in low-resource regions, and finally the prospects for very low cost handheld hyperspectral imaging instruments. A list of further reading and links to review articles was also included. I also included the discussion on heterogeneity and detection limits from the Photonics Spectra article. If you listen to this, please let me and Photonics Spectra know your reactions and questions.

Contributed by Richard Crocombe
Crocombe Spectroscopic Consulting

A typical "cordless drill" form factor handheld instrument, Vanta portable XRF from Olympus. (Picture courtesy of Olympus)

A typical "paperback book" form factor handheld instrument, NanoRam portable Raman from B&WTek. (Picture courtesy of B&WTek)

Do you have something spectroscopy-related you want to discuss in the newsletter?
Or something that will help our membership such as career tips or application tips?
Please let us know by emailing xchen4@dow.com.

Telephone: 301-694-8122
FAX: 301-694-6860