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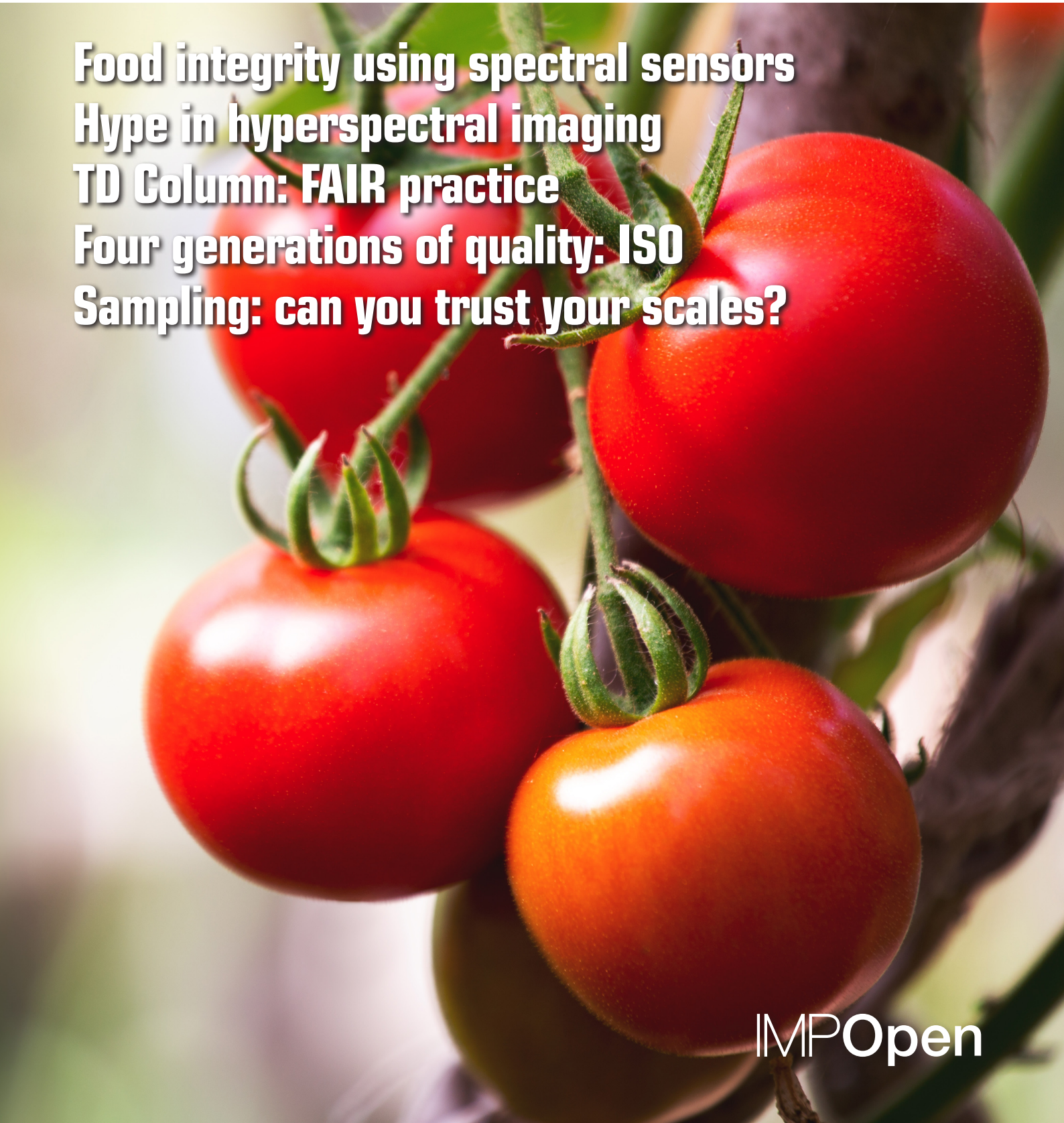

Food integrity using spectral sensors
Hype in hyperspectral imaging
TD Column: FAIR practice
Four generations of quality: ISO
Sampling: can you trust your scales?

IMPOpen

Food, food safety and food integrity are the reasons behind a new European COST Network investigating the use of non-destructive spectral sensors for these applications. The network is introduced by Lola Pérez-Marín in the article staring on page 15.

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IMPOpen

EDITORIAL

What we say and what we mean are not always the same! In science, accuracy in communication is of particular importance, which is one reason why reputable publishers spend so much time and money on copy editing papers. Clarity is of particular importance when the technology being described crosses boundaries between disciplines. It is surprising, to me at least, how often terminology can have quite different meanings in different communities.

Early in 2020, we published a paper in *Journal of Spectral Imaging* titled "The hype in spectral imaging", which we are reprinting in this issue. It raises questions about the terminology used to describe the combination of imaging and spectroscopy. This is not just pedantry, clarity is important. I would urge all readers involved in the fields of "imaging spectroscopy" and "spectral imaging" to have their say. You can use the commenting facility on the web-based version of the article, contact the authors or send your thoughts to me (ian@impopen.com) for potential publication.

Our second article describes a new European initiative to apply non-destructive sensors for food integrity. I anticipate that we will see low-cost instruments come out of this network that can have a significant impact on our food supply. Lola Pérez-Marín is Chair of SensorFINT, which welcomes the cooperation of other individuals and organisations.

FAIRness remains on Tony Davies' mind and his column looks at recent examples of the practical application of the FAIR initiative for research data. It may mean significant changes for all those involved in research, from funders, through researchers themselves to publishers of the results. However, the potential rewards are great!

John Hammond continues his mini series of columns looking at four generations of quality with a look at the impact of the International Standards Organization (ISO).

Kim Esbensen is joined by Aldwin Vogel to continue his discussion of sampling errors. They describe how sampling and weighing are different, but the same! The column focuses on weighing errors in detail, adding essential theoretical elements and practical know-how to the framework of the Theory of Sampling.

John Hammond appears again in a new section, "The Lighter Side". This aims to publish short and amusing or novel stories from you! It is something I have been "toying" with for decades, so I am most grateful to John for putting his story forward. If you have a memory of an amusing incident from the past, or just the other day, please do send it to me and I would be delighted to consider it for The Lighter Side.

NEWS

The world's most expensive egg timer?

A team of scientists has been using DESY's X-ray source PETRA III to analyse the structural changes that take place in an egg when you cook it. The work reveals how the proteins in the white of a chicken egg unfold and cross-link with each other to form a solid structure when heated. Their innovative method can be of interest to the food industry as well as to the broad field of research surrounding protein analysis. The work was the cooperation of two groups, headed by Professor Frank Schreiber from the University of Tübingen and Professor Christian Gutt from the University of Siegen, with scientists at DESY and European XFEL.

Eggs are among the most versatile food ingredients. They can take the form of a gel or a foam, they can be comparatively solid and also serve as the basis for emulsions. At about 80 °C, egg white becomes solid and opaque. This is because the proteins in the egg white form a network structure. Studying the exact molecular structure of egg white calls for energetic radiation, such as X-rays, which is able to penetrate the opaque egg white and has a wavelength that is no longer than the structures being examined.

"To understand the structural evolution in detail, you have to study the phenomenon on the micrometre scale", explains Dr Nafisa Begam, the lead author of the first study, who is an Alexander von Humboldt fellow in Schreiber's group. The scientists used X-ray photon correlation spectroscopy (XPCS) with a specific geometry allowing them to determine the structure and the dynamics of the proteins in the egg white.

For their experiments on the P10 beamline at PETRA III the scientists used a chicken egg from a supermarket and filled the egg white into a quartz tube of 1.5 mm diameter. "Inside, the egg white was heated in a controlled manner while we analysed it with the help of the X-rays", explains DESY co-author Fabian Westermeier. "The X-ray beam was expanded to 0.1 by 0.1 mm, to keep the radiation dose below the damage threshold of the protein structures."

The measurements reveal the protein dynamics in the egg white over a period of about a quarter of an hour. During the first three minutes, the protein network grew exponentially, reaching a plateau after about five minutes, at which virtually no more protein links were formed. At this time, the average mesh size of the protein network was about 0.4 µm.

In the second study, the team used the XPCS technique to investigate the self-organisation of protein solutions into domains with, respectively, high and low protein concentration, as an example of structure formation in cell biology. In the process, they were able to follow the temperature-dependent dynamics over time. "At high protein densities, mobility decreases, which slows down the phase separation. This is important for the special dynamics of the system", reports lead author Anita Girelli from Schreiber's group.

The studies not only reveal new details about the structural changes occurring in egg whites, but also prove the experimental concept, which can be used for other samples too, as demonstrated by the second study. "Successfully applying X-ray photon correlation spectroscopy opens up a new way to study the dynamics of biomolecules, which is essential if we are to understand them properly", Schreiber comments.

See their paper in *Physical Review Letters* (doi.org/fx9f).

LC-MS of skin swab samples detect COVID-19

The most widely used approach to testing for COVID-19 requires a polymerase chain reaction (PCR) test, which involves taking a swab of the back of the throat and far inside the nose. New research by chemists from the University of Surrey, Frimley NHS Trust and the Universities of Manchester and Leicester involved the collection of sebum samples from 67 hospitalised patients—30 who had tested positive for COVID-19 and 37 who had tested negative. The samples were collected by gently swabbing a skin area rich in sebum, such as the face, neck or back. The samples were analysed by liquid chromatography mass spectrometry (LC-MS) and partial least squares-discriminant analysis (PLS-DA) to differentiate between the COVID-19 positive and negative samples.

The Surrey team then found that patients with a positive COVID-19 test had lower lipid levels, or dyslipidemia, than their counterparts with a negative test. The accuracy of the study's results increased further when medication and additional health conditions were controlled.

Dr Melanie Bailey, co-author of the study from the University of Surrey, said: "Unfortunately, the spectre of future pandemics is firmly on the top of the agenda for the scientific community. Our study suggests that we may be able to use non-invasive means to test for diseases such as COVID-19 in the future—a development which I am sure will be welcomed by all."

Matt Spick, co-author of the study from the University of Surrey, said: "COVID-19 damages many areas of metabolism. In this work, we show that the skin lipidome can be added to the list, which could have implications for the skin's barrier

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function, as well as being a detectable symptom of the disease itself."

Dr George Evetts, Consultant in Anaesthesia & Intensive Care Medicine at Frimley Park Hospital, said: "Investigating new methods of diagnosis and surveillance in a new disease such as COVID-19 that has had such a devastating effect on the world is vital. Sebum sampling is a simple, non-invasive method that shows promise for both diagnostics and monitoring of the disease in both a healthcare and a non-healthcare setting."

The work was published in *Lancet E Clinical Medicine* (doi.org/fzwt).

MS protein fingerprinting in minutes

Researchers from Charité-Universitätsmedizin Berlin and the Francis Crick Institute have developed a mass spectrometry-based technique capable of measuring samples containing thousands of proteins within just a few minutes. It is faster and cheaper than a conventional blood count. To demonstrate the technique's potential, the researchers used blood plasma collected from COVID-19 patients. Using the new technology, they identified 11 previously unknown proteins which are markers of disease severity.

The researchers have developed a data-independent acquisition method, "Scanning SWATH", that increases the mass spectrometer's duty cycles. Developed under the leadership of Professor Dr Markus Ralser, Director of Charité's Institute of Biochemistry, this technology, which is much faster and cost-effective than previous methods, enables researchers to measure several hundred samples per day.

"In order to speed up this technology, we changed the mass spectrometer's electric fields. The data produced are of such extreme complexity that humans can no longer analyse them", explains Einstein Professor Ralser, who is also a Group Leader at the Francis Crick Institute in London. He adds: "We therefore developed computer algorithms that are based on neural networks and which use these data to extract the relevant biological information. This enables us to identify thousands of proteins in parallel and greatly reduces measuring timescales. Fortunately, this method is also more precise."

This high-throughput method has a broad range of potential applications, ranging from basic research and large-scale drug development to the identification of biomarkers, which can be used to estimate an individual patient's risk. This was demonstrated by the researchers' study on COVID-19. As part of this research, the team analysed blood plasma samples from 30 Charité in-patients with COVID-19 of varying degrees of disease severity, comparing the protein patterns obtained with those of 15 healthy individuals. The actual measurements conducted on individual samples only took a few minutes.

The researchers were able to identify a total of 54 proteins whose serum levels varied according to the severity of COVID-19. While 43 of these proteins had already been linked to disease severity during earlier studies, no such relationship had been established for 11 of the proteins identified. Several of the previously unknown proteins associated with COVID-19 are involved in the body's immune response to pathogens which increases clotting tendency. "In the shortest of timeframes, we discovered protein fingerprints in blood samples which we are now able to use to categorise COVID-19 patients according to severity of disease", says one of the study's lead authors, Dr Christoph Messner, who is a researcher at Charité's Institute of Biochemistry and the Francis Crick Institute. He continues: "This type of objective assessment can be extremely valuable, as patients will occasionally underestimate the severity of their disease. However, in order to be able to use mass spectrometry analysis for the routine categorisation of COVID-19 patients, this technology will need to be refined further and turned into a diagnostic test. It may also become possible to use rapid protein pattern analysis to predict the likely course of a case of COVID-19. While the initial findings we have collected are promising, further studies will be needed before this can be used in routine practice."

Professor Ralser is convinced that mass spectrometry-based investigations of the blood could one day complement conventional blood count profiles. "Proteome analysis is now cheaper than a complete blood count. By identifying many thousands of proteins at the same time, proteomic analysis also produces far more information. I, therefore, see enormous potential for widespread use, for instance in the early detection of diseases. We will, therefore, continue to use our studies to develop proteome technology for this type of application."

Read more in the paper in *Nature Biotechnology* (doi.org/f5x3).

Photo by Aaron Burden on Unsplash

Plastic pollution in snow

As snow melts it can leave pollution behind in the form of micro- and nanoplastics according to a study from McGill University. The pollution is largely due to the relatively soluble plastics found in antifreeze products (polyethylene glycols) that can become airborne and picked up by the snow.

The researchers have developed a new nanostructured laser desorption/

ionisation time-of-flight mass spectrometry (NALDI-TOF-MS) technique to analyse snow samples collected in April 2019 in Montreal for both micro- and nano-sized particles of various plastics. The NALDI-TOF-MS technique is orders of magnitude more sensitive than any of the other current methods used for tracing plastic in the environment. It allows scientists to detect ultra-trace quantities (pg levels) of many of the most common soluble and insoluble plastics in snow, water, rainfall and even in soil samples once they have been separated.

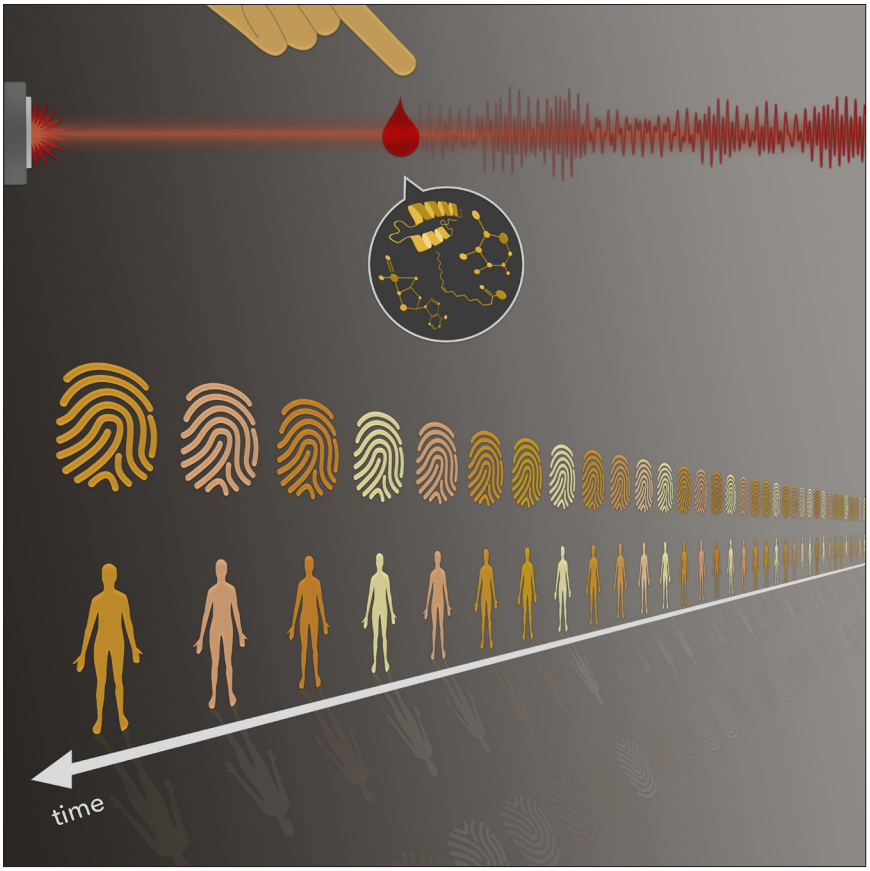
"It is important to be able to detect even trace quantities of plastics in the environment", says senior author, Parisa Ariya, from McGill's Departments of Chemistry and Atmospheric and Oceanic Sciences. "Though these plastics may be harmless in themselves, they can pick up toxic organic matter and heavy metals from the environment, which can damage human cells and organs."

Zi Wang, a PhD Candidate at McGill adds, "Our hope is that this new technique can be used by scientists in different domains gain key information about the quantity of micro- and nano-plastics in urban environments in order to better address their impacts on the ecosystem and on human health."

Find out more in *Environmental Pollution* (doi.org/f5zc).

Innovative blood test based using FT-IR

The molecular composition of blood provides information regarding a person's health and may be compared to an individual fingerprint. In principle, changes in the constituents of blood can serve as early signs of disease. However, before chemical fingerprints can be utilised for diagnostic purposes, the stability of the molecular patterns in healthy persons over time must be firmly established. Researchers under the direction of Dr Mihaela Žigman, Head of the Broadband Infrared Diagnostics (BIRD) group in the Department of Laser Physics led by Professor Ferenc Krausz at LMU Munich and the Max Planck Institute of Quantum Optics (MPQ), in collaboration with Professor Dr Nadia Harbeck at the LMU Medical Centre, have now successfully accomplished this. With the aid of Fourier-transform infrared (FT-IR) spectroscopy, the team has shown that the molecular composition of blood samples obtained from a cohort of healthy donors remains stable over a period of several months, and confirmed that each of the resulting spectra could be clearly assigned to an individual person.



Blood panels are as individual as fingerprints. Researchers from the attoworld team at LMU and MPQ have now investigated how stable this so-called molecular fingerprint of the blood is over time.

Rapid diagnosis of human diseases is a long-standing problem in medicine. As diseases often alter the molecular make-up of circulating body fluids, obtaining a snapshot of their molecular composition would be invaluable in detecting a multitude of diseased states, and the types and concentrations of the many molecules found in the bloodstream can provide vital information on a person's health. The real challenge, however, comes when one tries to determine the exact composition of body fluids, given that the concentrations of informative molecules are often extremely low. The interdisciplinary BIRD team has now investigated the stability of the chemical make-up of blood samples over days, weeks and even months.

Based on FT-IR measurements, the researchers analysed the molecular fingerprints of serum and plasma samples obtained from 31 healthy individuals over the clinically relevant period of 6 months. The study demonstrated that the IR molecular fingerprint of each individual donor remained stable over

periods ranging from a few days to weeks and months, and each temporal profile could be readily attributed to the participant concerned.

"This newly revealed temporal stability of blood-based infrared fingerprints provides a basis for future applications of minimally invasive infrared spectroscopy as a reliable method for the future of health monitoring", says Mihaela Žigman, leader of the research group.

Standard FT-IR spectroscopy could soon use infrared lasers as the source and, given the much higher intensity of laser light, this should yield more detailed and informative characterisations of the molecular constituents of blood. Physicists in the attoworld team, led by Professor Ferenc Krausz, are now working on the laser technologies necessary to achieve this. As Professor Krausz and colleagues reported last year, the new method allows minuscule amounts of different classes of molecules to be spectroscopically detected (*Nature*, doi.org/gg9z63).

"With our lasers, we can already detect electrical signals emitted by excited molecules with very high sensitivity", Ferenc Krausz explains. "Such precise measurements of alterations in the molecular composition of body fluids, together with knowledge of the stable molecular fingerprint of healthy controls, opens up new analytical opportunities in biology and medicine", says Marinus Huber, lead author of the study. "Our results reveal that it is possible to obtain informative, blood-based infrared fingerprints efficiently, repeatedly and in a minimally invasive manner. The key, in this case, is that the analysis ought to be sensitive enough and sufficiently broad to cover a wide range of possible molecules (or types of molecules)—to be in position to monitor personal health and detect disorders at an early stage. Practically speaking, following-up a person's health status regularly might become paramount for timely-detecting relevant deviations. In addition to its uses in the fields of health monitoring and preventive medicine, systems biology shall also benefit from the availability of the approach", Mihaela Žigman adds.

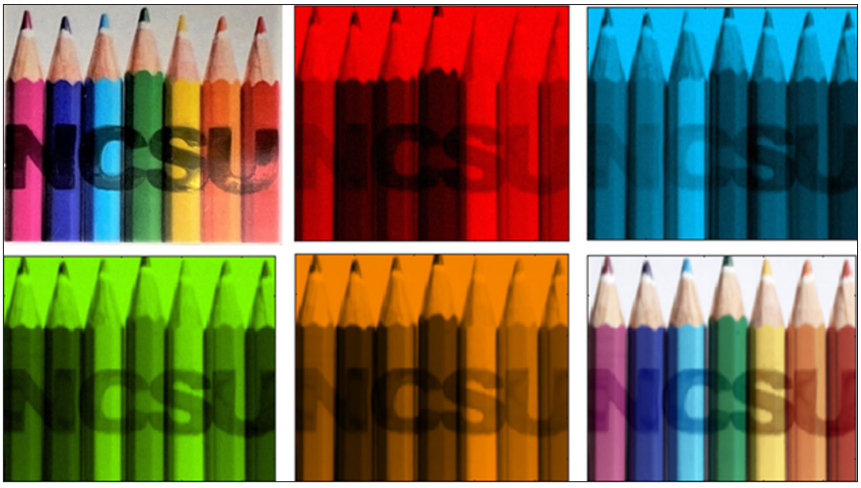
More information in *Nature Communications* (doi.org/gjhcq4).

Hyperspectral shrimp

"Lots of artificial intelligence (AI) programs can make use of data-rich hyperspectral and polarimetric images, but the equipment necessary for capturing those images is currently somewhat bulky," says Michael Kudenov, co-corresponding author of a paper on the work, *Science Advances* (doi.org/gjgcf6), and an associate professor of electrical and computer engineering at North Carolina State University. "Our work here makes smaller, more user friendly devices possible. And that would allow us to better bring those AI capabilities to bear in fields from astronomy to biomedicine."

While there are larger devices that are capable of capturing hyperspectral and polarimetric images, smartphone-sized imaging technologies have run into significant challenges. For example, the design of cell phone camera technologies results in very slight errors in the alignment of the different wavelengths of light in the final image. And the problem is exacerbated when a camera can capture more wavelengths, as is the case with hyperspectral technologies.

The creators of the new light sensors were inspired by the eyes of mantis shrimp, which are exceptionally good at accurately capturing subtle gradations of colour. So, the researchers created an organic electronic sensor that mimics the mantis shrimp's eye. Its called the Stomatopod Inspired Multispectral and POLarisation sensitive (SIMPOL) sensor. The researchers developed a prototype SIMPOL sensor that can simultaneously register four spectral channels and three polarisation channels. While only a proof of concept, the researchers used modelling simulations to determine that the design could be used to create detectors capable of sensing up to 15 spatially registered spectral channels.



This SIMPOL image shows spectral imaging of a scene containing objects with different colours, as well as the letters NCSU, which contain different polarisation states. Image credit: Ali Altaqui.

"SIMPOL's colour channels can discern spectral features 10 times narrower than typical imaging sensors; in other words, it is 10 times more precise", Kudenov says.

"Our work demonstrates that it is possible to create small, efficient sensors that can simultaneously capture hyperspectral and polarimetric images", says Brendan O'Connor, co-corresponding author of the paper and an associate professor of mechanical and aerospace engineering at NC State. "I think this opens the door to a new breed of organic electronic sensing technologies."

Infrared microscopy goes "off grid"

Researchers from Caltech, UC Berkeley and the Berkeley Synchrotron Infrared Structural Biology Imaging Program (BSISB) have reported a more efficient way to collect "high-dimensional" infrared images. With the new method, scans that would have taken up to 10 hours to complete can now be done in under an hour, potentially broadening the scope of biological spectromicroscopy to time-sensitive experiments.

"We realised that sampling our model organism—the small roundworm *C. elegans*—as it changes over time was challenging for software rather than hardware reasons", said Elizabeth Holman, a graduate student in chemistry at Caltech. "For example, image sampling was limited to uniform-grid raster scans with rectangular boundaries and fixed distances between sample points."

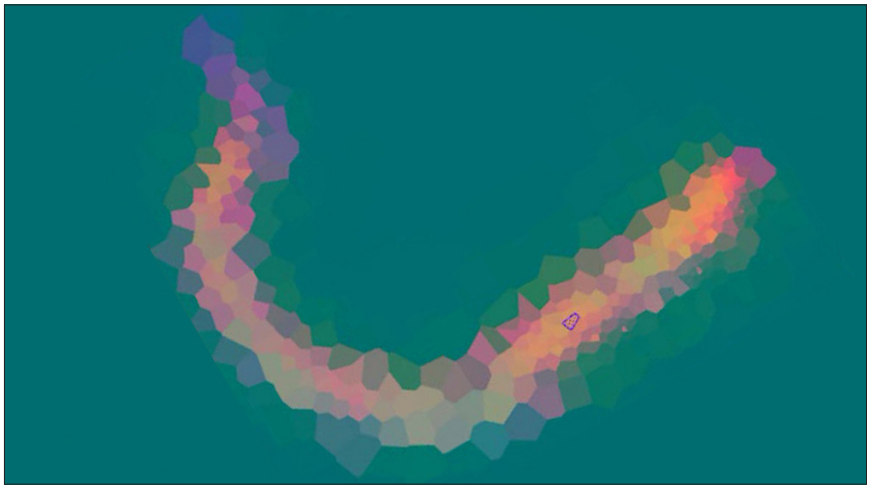
The new technique, implemented at the ALS with Yuan-Sheng Fang, a graduate student in physics at UC Berkeley, uses a grid-less, adaptive approach that autonomously increases sampling in areas displaying greater physical or chemical contrast. In the proof-of-concept infrared microscopy experiments, the researchers examined two samples.

The first was a two-component system in which both components (permanent-marker ink and high-vacuum grease) were well characterised. Details of the sample were very difficult to see clearly with the naked eye, so it was a good test of how the software would perform with minimal guidance from a human experimenter. The second sample was a live, larval-stage *C. elegans*, a biological model system studied by thousands of researchers.

In both cases, autonomous adaptive data acquisition (AADA) methods clearly outperformed non-adaptive methods. In the second example, increased sampling density corresponded with known *C. elegans* anatomical features, and the head region was mapped in 45 min as opposed to about 4.9 h using commercially available software.

"Outside of our specific published work, the results suggest that integrating AADA into existing scanning-based satellite, drone and/or microscope techniques can facilitate research in fields ranging from hyperspectral remote sensing to ocean and space exploration", said Holman.

The research has been published in *Communications Biology* (doi.org/f5x8).



Example of the tiling pattern used in scanning a *C. elegans* roundworm. The non-grid-based pattern gives the sampling algorithm greater flexibility to quickly zero in on areas of interest. (Credit: Elizabeth Holman/Caltech and Yuan-Sheng Fang/Berkeley Lab)

NEWS

Company News

MS data analysis for biopharma and proteomics

Thermo Fisher Scientific and Protein Metrics have entered into a non-exclusive co-marketing agreement to provide advanced mass spectrometry data processing and analysis capabilities for biopharmaceutical and proteomics applications, from research and development to quality control. Thermo Fisher brings the cloud-enabled Thermo Scientific Chromeleon CDS software to the collaboration, which will work with Protein Metrics' Byos platform for protein characterisation that allows post-translational modifications and other critical quality attributes to be monitored.

NMR platform for metabolomics-based, AI-driven diagnostics

numares AG has made a 510(k) submission to the US Food and Drug Administration (FDA) for its AXINON® IVD System, a NMR-platform for AI-driven, metabolomics-based diagnostics. If cleared, AXINON® would become the first NMR-based clinical laboratory system using AI-evaluated metabolic data. Several multi-marker assays for AXINON® will cover numerous unmet medical needs for preventing, diagnosing and treating disease.

numares is currently developing multi-marker algorithms for several diagnostic tests on the AXINON® IVD System. These include AXINON® GFRNMR to reliably assess kidney function by improved determination of glomerular filtration rate (GFR). numares expects to submit this test to the FDA also in the first half of 2021. The third assay AXINON® renalTX-SCORE® is intended to reliably identify early kidney rejection in post-transplant surveillance, and be submitted to the FDA in 2022. Further multi-marker tests are in development, e.g., for liver disease, cancer detection and multiple sclerosis.

NIR-HSI for quantitative detection of fatty liver disease

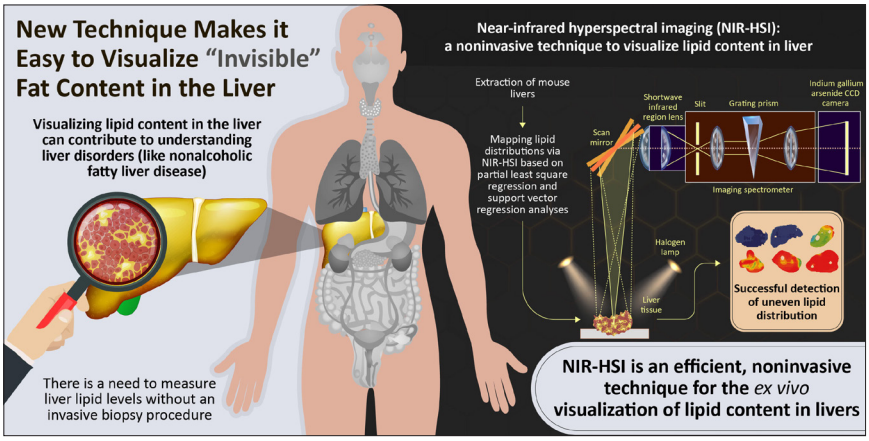
Non-alcoholic fatty liver disease (NAFLD) is a pathological condition characterised by excessive fat stored in the liver that is not attributed to heavy alcohol consumption, which can lead to liver failure and even cancer. Obesity, type 2 diabetes and high cholesterol levels are all risk factors for this disease, and like the global prevalence of obesity, the prevalence of NAFLD is coincidently expected to rise as well.

It is, therefore, critical for clinicians to have effective tools for diagnosing NAFLD. The current standard method for diagnosis is analysis of liver biopsy samples. However, this approach has shortcomings such as invasiveness and the potential for sampling errors, so there is a pressing need for reliable non-invasive methods. In a new study, a team of researchers, led by Professor Kohei Soga of Tokyo University of Science including Assistant Professor Kyohei Okubo of Tokyo University of Science and Professor Naoko Ohtani of Osaka City University, reports the successful use of near infrared hyperspectral imaging (NIR-HSI) to quantitatively analyse the distributions of lipids in mouse liver. Dr Okubo says, "Lipid distribution in the liver provides crucial information for diagnosing fatty liver-associated liver diseases including cancer, and therefore, a non-invasive, label-free, quantitative modality is needed."

The study focused on mice that were either on a normal diet or one of three kinds of high-fat diets rich in various types of lipids. The objective of these varied diets was to generate a set of livers with diverse lipid profiles. After extracting the livers, the scientists used a reference test to generate accurate results to compare their HSI results to. They used the Folch extraction method to isolate lipids from small pieces of the livers and then weighed the isolated lipid samples to calculate the total weight of lipids within the livers. NIR-HSI was then performed and two candidate data analysis methods—partial least-square regression and support vector regression—were used to quantitatively visualise lipid distributions within the liver to identify the better analytical method.

The lipid levels as measured with HSI closely correlated with the actual lipid levels as quantified by the Folch extraction method, and this correlation was stronger in the lipid levels calculated using support vector regression than for the lipid levels calculated using partial least square regression.

Dr Okubo highlighted the significance of his team's research, "We have developed a method to visualise the distribution of lipids in the liver using a near infrared spectral imaging technique that incorporates machine learning." This is important because NIR-HSI allows non-invasive evaluation of the liver status, thus providing a diagnostic option for clinicians when investigating NAFLD cases. NIR-HSI can also be used to detect specific types of lipids, and Dr



Courtesy of Tokyo University of Science

Okubo emphasised that "the ultimate goal of this collaborative research is to differentiate and identify fatty acids in the liver". Achieving this future goal would represent a major advance in research in fatty liver diseases, *Biomedical Optics Express* (doi.org/f5zb).

Direct observation of charge separation in an organic light-harvesting system

Molecular heterojunctions receive significant attention due to their key role in a wide variety of emerging organic semiconductor applications, such as organic light-emitting diodes, field-effect transistors, spintronic devices and photovoltaic cells. Understanding ultrafast dynamics of photon-to-charge conversion is paramount for optimising novel light-harvesting systems. By using the femtosecond long X-ray pulses of the free-electron laser FLASH at the plane-grating monochromator beamline PG2 and the wide-angle electron spectrometer (WESPE) end station, a team of researchers has access to specific charge separation sites and monitor free charge formation in a model donor–acceptor system on their natural timescale.

The basic principle of time-resolved X-ray photoemission spectroscopy (TR-XPS) is the combination of two light pulses, whereas a "pump" pulse initiates electronic dynamics inside the sample and their time evolution is monitored by a second, delayed X-ray "probe" pulse. The sample was excited with optical laser pump pulses with a wavelength of 775 nm and used photons generated by FLASH as probe pulses with a wavelength of 7.5 nm (3rd harmonic).

The carbon 1s core level XPS signal reveals the specific atomic sites where charges are located. A previously unobserved channel for electron-hole pair (exciton) dissociation into mobile charge carriers is identified, providing the first direct, real-time characterisation of the timescales and efficiency of charge generation in an organic heterojunction. The team of scientists from TU Bergakademie Freiberg, DESY, European XFEL and Lawrence Berkeley National Laboratory in Berkeley (US) demonstrate that the previously reported lifetime of interfacial charge-transfer (ICT) states of ~1 ps results from the competition between two separate relaxation channels: interfacial electron-hole recombination and ICT dissociation into delocalised charges.

Moreover, the data provide direct access to the efficiency for free charge carrier generation from ICT states at the CuPc-C60 interface. The TR-XPS technique has long been hailed as a potential candidate to address some of the most pressing questions regarding light-to-charge conversion in condensed phase systems. This work, however, is the first demonstration that it indeed provides otherwise unattainable information regarding the key steps of these processes by monitoring the birth of delocalised charges from tightly bound ICT states in a canonical model system for organic heterojunctions.

Furthermore, the findings give strong support to the emerging realisation that charge separation, even from energetically disfavoured excitonic states, is contributing significantly, indicating new options for light harvesting in organic heterojunctions. The direct determination of energetics, temporal dynamics and relative channel efficiencies for an archetypical organic heterojunction hold great promise that other light-harvesting processes in complex, multi-compound systems may be studied on their natural timescales. The unprecedented site-specificity provided by ultrafast TR-XPS at FLASH paves the way towards a better understanding of novel photovoltaic and photocatalytic frameworks.

The results were published in *Nature Communications* (doi.org/fz5k).

Gordon F. Kirkbright and Edward Steers Bursary Awards 2022

The Gordon F. Kirkbright bursary award is a prestigious annual award that assists a promising early career scientist of any nation to attend a recognised scientific meeting or visit a place of learning. The fund for this bursary was established in 1985 as a memorial to Professor Gordon Kirkbright in recognition of his contributions to analytical spectroscopy and to science in general.

Owing to the generosity of one of our former trustees, an eminent atomic spectroscopist, Professor Edward B.M. Steers, we are now able to award an annual Edward Steers bursary, in addition to the long-standing Gordon Kirkbright bursary, to similarly assist a promising early scientist engaged in or utilising analytical spectroscopic techniques.

The ABS Trust defines early career as being either a student, or an employee in a non-tenured academic post or in industry, within seven years of award of PhD excluding career breaks. The same conditions apply to each bursary.

Applications are invited for both the 2022 Gordon Kirkbright Bursary and the 2022 Edward Steers Bursary. Although both funds are administered by the ABS Trust, the Kirkbright award is not restricted to spectroscopists, but is open to all involved with or utilising analytical science-based techniques.

Application Forms can be downloaded via http://www.abstrust.org/kirkbright-and-steers-bursary-awards or for further information visit http://www.abstrust.org or contact abstrustuk.kirkbright@gmail.com

The closing date for entries is 30 November 2021.

ARTICLE

The hype in spectral imaging

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Hyperspectral imaging is currently a very well-known and much used technology for measuring features in different fields, such as chemistry, geology, medicine, food and agriculture, either spaceborne (satellites), airborne (drones) or at close proximity (e.g. field scanning, industrial sorting lines or microscopy). Its background is two-fold, and it can be considered as a special case of spectroscopy ("imaging spectroscopy") or a special case of imaging ("spectral imaging"). Current practice is to use adjectives such as multi and hyper added to "spectral imaging" in order to characterise the number of wavelength bands. In this paper we propose the community to use scientifically sound terminology, like "imaging spectroscopy" or "spectral imaging", without using ambiguous adjectives. Further, we encourage the community to define and agree upon clear adjectives to describe the number of variables in the naming of our imaging technique.

Historical notes

Spectroscopy has its origin in the 17th century when Isaac Newton demonstrated that white light from the sun could be dispersed into a continuous series of colours, coining the word spectrum to describe this phenomenon. Later, Kirschoff and Bunsen[1] found a relationship between the chemicals and the specific spectrum of light emitted when gases are burned. Traditionally, single ("point") spectra are measured within a single spatial region, however, this technique has been extended to scanning multiple spectra in a spatial preserving way, resulting in imaging spectroscopy. Conversely, spectral imaging finds its background in imaging. The first photographs only depicted different values of grey, where a pixel's grey value denotes the light reflection over the whole visible spectrum. In colour imaging, each pixel consists of a red, green and blue pixel, similar to the light receptors in a human eye. By extending the number of wavebands per pixel the technique of spectral imaging was born.

The term "hyperspectral imaging" originated in the mid-1980s from the remote sensing community with the development of the Airborne Imaging Spectrometer (AIS) at NASA's Jet Propulsion Lab, an airborne instrument capable of imaging large regions of the Earth in the short-wavelength infrared (SWIR) wavelength range (1200–2400 nm).[2,3] The subsequent development of NASA's Airborne Visible/Infrared Imaging Spectrometer (AVIRIS) expanded the application of spectral imaging to a wide range of tasks, from vegetation monitoring to mineral mapping on the Earth's surface. The term "imaging spectroscopy" is now preferred over "hyperspectral imaging" by NASA.[4] However, use of the term "hyperspectral imaging" has persisted and grown in both the scientific and non-scientific vernacular. Indeed, a recent paper title search in Web of Science indicates that in excess of three times more articles have been published in the past 10 years with the words "hyperspectral imaging" in the title than with "imaging spectroscopy". Figure 1 depicts the number of hits for both terms as function of time. From this graph we clearly see that although "imaging spectroscopy" is used much earlier than "hyperspectral imaging", the latter increased exponentially and overtook "imaging spectroscopy" in 2005.

Discussion

Currently, it is common practice to subdivide spectral imaging into multispectral imaging for images with a few waveband values and hyperspectral imaging for images composed of hundreds of waveband values. In our opinion this subdivision is prone to subjectivisms, which is proven by the fact that some papers use "multispectral" for images with 25 wavebands[5] while others use "hyperspectral" for the same number of wavebands.[6] In the literature "hyperspectral" mainly is related to imaging, but there are a few examples where "hyperspectral analysis" refers to plain spectroscopy,[7] adding further ambiguity to the term. To make it even more confusing sometimes "superspectral" is used for 10–20 bands.[8,9] The question also arises: what's beyond hundreds of wavebands? In literature, the term "ultraspectral" is used for images with

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512 wavebands[10] while others use it for images with more than 2000 bands.[11]

Although with regard to the processing of data envisaged in publications, indicating the number of spectral variables in the name of the imaging technique has its advantages. For example: the complexity of the algorithms and the suitability of different analysis approaches (e.g. chemometrics, image analysis or hybrid approaches) may differ according to the number of wavebands. Nevertheless, the use of ambiguous terms, as mentioned above, does not contribute to the clarity of the research publications.

A side effect of using the term hyperspectral imaging is that often the term hypercube is used as a reference to hyperspectral image data. From a Web of Science search over the period 2015–2019, we found 38 articles having "hyperspectral" in the title that mentioned the term "hypercube" in the title, abstract or keywords. A typical example is the development of convolutional sparse coding techniques for hyperspectral images.[12]

In geometry, a hypercube is an *n*-dimensional analogue of a square ($n=2$) and a cube ($n=3$).[13] Spectral image data in general is a three-dimensional array with spatial information in the first two dimensions and spectral information in the third dimension (Figure 2). It is seldom a cube, as the spatial and spectral dimensions most often differ from each other. Therefore, hypercube is not a proper term to describe spectral image data.

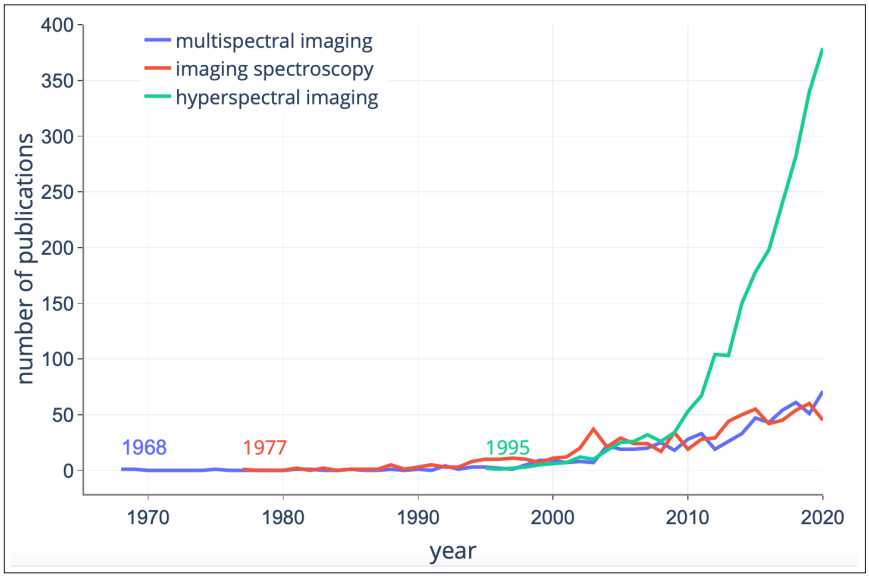

Figure 1. Web of Science title search hits for "hyperspectral imaging", "multispectral imaging" and "imaging spectroscopy". Updated from Reference 14.

Conclusion

To conclude, we propose that the community promote the use of scientifically sound terminology, such as "imaging spectroscopy" or "spectral imaging", without using exaggerated adjectives. Furthermore, we advise against the use of inappropriate terms, like hypercube for a three-dimensional (x,y,λ) data array or hyperspectral analysis for point spectroscopy.

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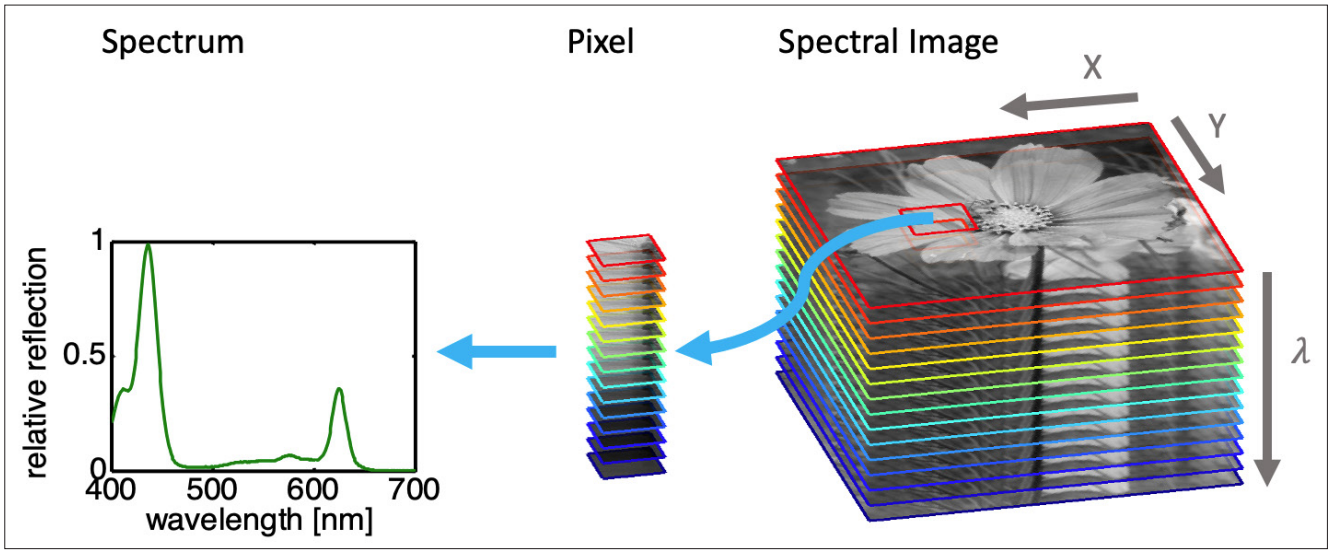

Figure 2. A spectral image depicted as three-dimensional data array.

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ARTICLE

SensorFINT, the new European Network for assuring food integrity using non-destructive spectral sensors

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The SensorFINT COST Action (CA19145) is a European Network for assuring food integrity using non-destructive spectral sensors. SensorFINT is funded by the European Cooperation in Science and Technology (COST) organisation with the primary objective of promoting the creation of research networks in innovative areas, facilitating the collaboration between academia and industry in Europe and beyond.

Our main objective is to create a vibrant and multidisciplinary network focused on the application of non-destructive spectral sensors to solve the demands of industry for assessment of the quality, safety, authenticity and traceability of food, combining experience in research, manufacture, training and technology transfer to accelerate spectral sensor implementation throughout the food chain. Thus, the Action is oriented to the use of sensors and technologies that allow the design of new, intelligent quality control systems to achieve the new challenges of Industry 4.0. That is, a widespread and instantaneous non-destructive inspection of food products to enable decisions to be taken in real time from "field to fork", providing a unique digital fingerprint of the product and, therefore, a new digital labelling strategy with a more complete information about the product for consumers.

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Currently, there is an increasing need for the food industry to provide information on their products in order to satisfy consumer demands, quality standards, to produce more and to protect their products from food fraud. Recent developments in technology, and advances in big data analytics, provide the opportunity for step-changes that can transform the role of food integrity assurance from one of just strictly conformance to one that addresses a wide range of business-critical concerns, including quality, safety and authenticity solutions. Non-Destructive Spectroscopic Sensors (NDSS), such as near infrared (NIR) spectroscopy, fluorescence, Raman or hyperspectral imaging, enable rapid, non-destructive and environmentally-safe assessment of multiple parameters in a variety of food products. Most applications of these technologies in the food industry are carried out in the laboratory. Nevertheless, industry requires them to be deployed *in situ*, i.e. on-line, in-line, on-farm, in-field, for full process control over the entire food chain. These requirements introduce constraints on sensor design and calibration development, which do not normally apply to laboratory-based instruments. Long-term stability of instruments, robustness of calibrations, sensor integration in production environments, transferability of data and the building of real-time decision-making systems are critical issues to be considered.

In this Action, specific consideration has been given to those topics, challenges or key issues in NDSS for research and innovation that are still unaddressed or, at least, only partially addressed, such as:

- The integration of several spectral sensors (NIR, fluorescence, Raman etc.), especially combined with imaging systems, to solve critical issues in the agro–food sector. Therefore, the Action tackles the scientific breakthroughs necessary for the fusion of NDSS so that they can be implemented in many parts of the food chain, regardless of the demonstrated development of each technology separately for different food applications.
- The role of NDSS for the widespread sampling of bulk products and batches, highlighting one of their main advantages, which has not yet been fully exploited, the possibility of reducing the sampling error and, therefore, the total analytical error, providing a more precise answer.
- The development of ready-to-use analytical systems, based on the integration and combination of low-cost, portable and miniature NDSS, and information and communication technologies (ICT) for process control and voluntary labelling, to guarantee the integrity and reputation of high added-value products.

ARTICLE

Figure 1. Kick-off meeting of SensorFINT via Zoom.

- The potential of NDSS as non-targeted methods for the individual control of a product item, providing a product fingerprint as a valuable tool for food authentication and fraud prevention.

The SensorFINT Action will manage these NDSS challenges for the demands of the food industry, advancing the state-of-the-art in the technologies and contributing to advances in NDSS applications. This will involve different strengths and expertise, turning innovative ideas and breakthroughs into new products, solutions and applications. The project is structured into five Working Groups:

1) NDSS for innovation in process control and labelling in the European food industry.
2) Innovation related to the integration of multiple NDSS methods for critical issues in food integrity.
3) Novel mathematical algorithms and methods for processing NDSS in real time.
4) Use of ICT in building decision support systems for the industrial implementation of NDSS.
5) Dissemination and exploitation.

Under the framework of SensorFINT, a range of activities (conferences, workshops, training schools, exchanges and other dissemination activities) will be organised and funded to promote the culture of NDSS, their implementation in industry and to train future researchers and specialists in the field.

The SensorFINT Action is an open network, now involving more than 30 countries and 150 researchers from Europe and beyond, and it still welcomes new researchers working on spectral sensors, data processing or ICT. Networking activities of the Action, without any doubt, will promote the exchange of information between European and International partners, the dissemination of results and the training of young researchers, who will convert scientific results into a reality that matches industrial needs.

The Action started officially at the beginning of October 2020 (Figure 1) and will continue for four years. More information on all the events being organised, the members of the Action, the travel grants (STSM, Short-Term Scientific Missions) and much more could be found on our website, www.sensorfint.eu (Figure 2). Also, you may follow us on social media (Twitter, Instagram, Linkedin or Facebook) and be updated daily with all the information about SensorFINT's activity.

My last message, please book for our First International SensorFINT Workshop "Smart Spectral Sensors for Agri-Food Quality and Process Control" that will be held in Porto (Portugal) from 16 to 17 September 2021: a must-attend event for the whole NDSS community.

Figure 2. The SensorFINT website.

Dr Lola Peréz-Marín, Full-Professor in the Faculty of Agriculture and Forestry Engineering, University of Cordoba, Spain, is a worldwide-recognised expert in the use of NIR sensors for food integrity assessment. President of the Educational Committee of ICNIRS and Member of the International Scientific Advisory Board of the Institute for Global Food Security, Queen's University Belfast, UK. Recipient in 2014 of the international Tomas Hirschfeld Award and in 2020 of the international Gerald S. Birth Award for her outstanding contribution in the field of NIR spectroscopy.
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TONY DAVIES COLUMN

FAIR practice

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Following our articles on the FAIR initiative, our esteemed editor Ian Michael was very keen that we looked at some examples of the FAIRification of data handling, collection and archiving.

Fortunately, this request coincided with a webinar featuring some subject leaders in this field called "FAIR Data: From principles to best practices" and hosted by MyScienceWork on 30 March 2021.[1,2]

FAIR data: from principles to best practices

MyScienceWork describes themselves as having a mission of democratising science. Sally Ekanayaka who hosted the workshop stated that…

"MyScienceWork is a technology company that provides a suite of advanced data-driven solutions for research institutions, scientific publishers and private-sector R&D companies. Fostering digital discoverability and collaboration, securing long term accessibility and reusability of research outputs, and maximising research impact is at the heart of the company's repository solutions…"

and as such they clearly have a major interest in helping drive forward initiative in the FAIR field.

The planned key takeaways from the workshop were:

- An overview of FAIR data publishing standards
- Ways of operating the FAIR principles within research activities
- The core requirements for trustworthy digital repositories

So, it looked like a good bet to start gathering information on people and projects that have carried out FAIRification work.

FAIR for (data) publishers

Erik Schultes, who has been working full time for the last three years on FAIR implementation strategies at the GO FAIR Foundation and whose background is in the data intensive biological sciences, led off. His presentation focused on FAIR publishing and asked the question "what is your FAIR Implementation Profile". Erik's talk delivered on the first two "Takeaway" bullet points above. First, he emphasised that the GO FAIR Foundation is working with lots of organisations in different fields or domains and, as such, is completely "standards" agnostic. They deliberately leave the choice of which standards to adopt to the individual domain specialists. GO FAIR's support in their different interactions is to help these organisations reach the highest level of FAIR possible, whilst keeping an eye on what other initiatives are delivering in order to help drive convergence.

In January, Erik and Jan Velterop published a call-to-arms for a network of academic publishers to come together and make some joint decisions on FAIRification in the academic publishers' sector through a GO FAIR Implementation Network structure.[3] He reminded the listeners about the GO FAIR guide on "how to Go FAIR" which breaks down the FAIRification process into essentially three stages which starts off with decisions by communities of practice on domain relevant community standards. GO FAIR support this process by initiating Metadata 4 Machines activities to bring together domain experts with FAIR Metadata Experts to produce reusable, domain-specific FAIR metadata schema (Figure 1). Particular emphasis is to try, whenever possible, to use already agreed standards and avoid re-inventing the wheel.

From the perspective of available tools, Erik pointed out the CEDAR Workbench, an Open-Source tool for generating metadata that describe scientific experiments. Just be warned though, I had never heard of this tool and on Googling it I was presented with some very fine solid wood tables, but better links to a vast amount of information on the CEDAR tools can be found in Reference 4! CEDAR is the acronym for the *Center for Expanded Data Annotation and Retrieval*, a collaboration lead by Mark Musen with Stanford Co-PIs from Stanford, Oxford, Yale and Northrop Grumman. Their mission is to develop information technologies that make authoring complete metadata sets much more manageable, and that facilitate using the metadata in further research. The Open-Source CEDAR Workbench was specifically built to help deal with the extremely poor state of metadata generation, a critical activity in the FAIRification process as we have documented. It consists of a set of Web-based tools covering acquisition, storage, search and reuse of metadata templates including the simple construction of metadata acquisition forms. The metadata generated using CEDAR templates are FAIR compliant and interoperable with Linked Open Data and retrievable in JSON, JSON-LD and RDF formats. A nice short video explaining the nature of CEDAR is

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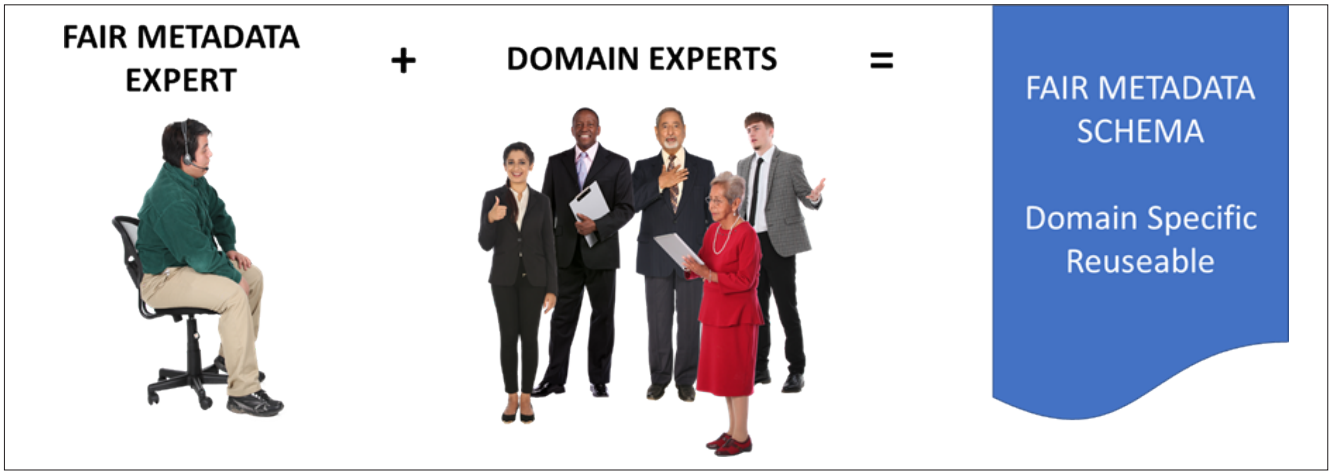

Figure 1. GO FAIR Metadata 4 Machines workshops are designed to bring domain experts and FAIR metadata experts together to generate domain-specific FAIR metadata schema.

available at https://more.metadatacenter.org/video/introductory-video-cedar-all-basics.

The creation of FAIR metadata is of course only part, even if a very important part, of the FAIRification process. The GO DATA FAIR Implementation Profile (FIP) concept which is the next step after the creation of the domain-specific metadata schema. At the time of writing there have been 25 FIPs created out of the FIP workshops and an article by Barbara Magagna from the Vienna Umweltbundesamt GmbH in Austria and co-workers from Prague and the Netherlands about the use of FIPs as accelerators for FAIR convergence is available currently on the OSF Preprints.[5]

Access to digital content—repositories

So, with the principles sorted the workshop moved on to the role of repositories and the core requirements of software to be capable of fulfilling this challenging role. Yann Mahe from the meeting hosts MyScienceWork took up the challenge of presenting concepts for data science solutions for research which can cope with the complexity and multidisciplinary nature of the content whilst satisfying the needs of diverse stakeholders. We have all observed the explosion of scientific data sources in the last 20 years, most of which has been outside of the classical peer-reviewed publishing model. In fact, it is probably fair to say that currently the majority of scientific data is "published" outside of the classical peer review quality control mechanism of the past. The COVID-19 pandemic has highlighted a real modern-day challenge facing data consumers in identifying and filtering out information that is either false or contextually extremely misleading in its presentation. Yann addressed the challenges to link, store and subsequently visualise this diverse "ocean" of data to which we all have access in a meaningful way.

The concept of Openness and Open Access in science gives huge potential opportunities for the scientific community. However, there can be gaps between the expectations of scientists regarding "Big Data" and the available tools for use and reuse. Such issues can inhibit obtaining the full benefit of the fundamental mould-breaking approach to science publication. Yann emphasised that the implementation of the FAIR principles is one solution to brining the expectations of researchers closer to fulfilment, but highlighted the different levels of progress between the early innovator countries and the rest of the world. This variation in support is not only reflected across the globe but also between individual scientific domains and communities who can be seen to have quite different concrete goals set by their stakeholders under the FAIR banner.

The essential role of repositories in collation, curation and presentation of data in a machine and human readable form was discussed. The fact that, in real-world operation, specific tooling meets multiple requirements around Findability, Accessibility, Interoperability and Reusability—a concept that the IUPAC FAIRSpec project is also confronting as it continues its domain-specific work.[6] Yann reviewed the concept of a repository especially around the role of repositories in lowering the barriers to the adoption of FAIR data principles whilst also generating additional connectivity to other related content both within the repository itself and between different repositories. This will greatly help mitigate the challenges around addressing different stakeholder demands.

For commercial entities, a well thought out repository is also essential in meeting underlying compliance and business critical drivers, such as around managing rights to finding and accessing specific content. There is also a need to deploy data retention policies, where data may be required to be deleted after a specific lifetime but also held should a legal hold be in place on the information content. Keeping systems future-safe also requires a well thought out end-of-life plan for any infrastructure and a well-managed FAIR repository is also far simpler to migrate to the next generation of software and hardware. Longevity is also ensured through implementing well-documented, controlled vocabularies within the repositories, which is where we come back to the work described by Erik above!

TONY DAVIES COLUMN

Deployment examples—from the Pistoia Alliance work in life science

The third workshop presentation was by Ian Harrow, Project Manager with the Pistoia Alliance based on the importance of the FAIR data initiative in the life sciences. Ian provided insights they have gained by building a toolkit for FAIR. Ian started off by reviewing the enormous growth in available data from the individual measurement through the move towards high-throughput methodologies, "omics" and now Big Data and the internet of things where data mining becomes essential and the FAIR guiding principles and data tools a key enabler. These tools and services also serve as a value multiplier for the available data, something worth remembering when you are trying to obtain funding your own projects! The FAIR principles are not a standard, but Ian pointed to the Research Data Alliance (RDA) FAIR Data Maturity Model published last year as a major step forward in "standardising" approaches to FAIRness.[7] There is a wealth of information on the RAD website at https://www.rd-alliance.org and if you are interested in learning more or contributing to their work there is the opportunity to join this organisation as a member or an organisation.

What is nice about the RDA approach is that it has looked at all the FAIR principles, which in their own right look quite daunting when starting out on your own FAIRification project and have assigned each one of three levels of importance.

The three levels of importance are defined as:

1) **Essential:** such an indicator addresses an aspect that is of the utmost importance to achieve FAIRness under most circumstances, or, conversely, FAIRness would be practically impossible to achieve if the indicator were not satisfied.
2) **Important:** such an indicator addresses an aspect that might not be of the utmost importance under specific circumstances, but its satisfaction, if at all possible, would substantially increase FAIRness.
3) **Useful:** such an indicator addresses an aspect that is nice-to-have but is not necessarily indispensable.

I see this as an excellent supporting document to help organisations develop and prioritise what Erik discussed under the GO FAIR FAIR Implementation Plan. Ian pointed out that the Pistoia Alliance had held three workshops in 2018 and 2019 in Europe and the USA which had clearly identified one of the major hurdles to FAIRification being "*just where do you start*"! It is clear that projects need to discuss and agree what are the underlying business goals and unambiguously document what does "FAIR Enough" mean in their worlds.

The Pistoia FAIR Toolkit arose to meet these needs recognising this needs to be a bottom-up approach and conceptualised their work around documenting use cases, identifying good tools, recognising the importance of training and the requirement across the whole work of good change management activities.[8,9]

With the space we have available it's impossible to go into the details of each individual project from birth to delivery that the alliance has run but if you follow the link in Reference 10 you will find five really interesting examples from Roche, Bayer, AstraZeneca, The Hyve and SciBite to go through.

Oddly enough, an old colleague Rolf Grigat who is now working at Bayer as a FAIR and Linked Data Enabler, had recently pointed me to the Bayer COLID implementation which is freely available on GitHub (https://github.com/Bayer-Group). He is particularly proud of their logo (Figure 2) and with any luck we will be able to feature in more detail the development journey that Bayer and the Pistoia Alliance took in a future column.

Figure 2

Conclusions

The timing workshop could not have been better. Covering concepts for FAIR deployments through systems to real-world examples of completed projects it really took the FAIRification idea forward from theory to real-world deployments. If you are still finding lockdown stressful why not take an hour out to listen to the whole workshop? You can use the link in Reference 1.

Everyone please, stay safe!

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TONY DAVIES COLUMN

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QUALITY MATTERS

Four generations of quality: International Standards Organization (ISO)

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Introduction

This article concentrates on the International Organization for Standardization (ISO) organisation, its standards and their place within the Quality environment. By definition, it discusses the role of ISO in the administration and control of these standards and their evolution and harmonisation into the standards currently in existence. This article will not discuss the specific application of ISO/IEC 17025 and ISO 17034 in association with ISO/REMCO, and accreditation authorities in the implementation of these standards; this aspect will be covered in the next article in the series.

ISO—Background and organisational structure

ISO is an international standard-setting body composed of representatives from various national standards organisations.

ISO is an independent, non-governmental organisation, the members of which are the standards organisations of the 165 member countries. It is the world's largest developer of voluntary international standards and it facilitates world trade by providing common standards among nations. More than 20,000 standards have been set, covering everything from manufactured products and technology to food safety, agriculture and healthcare.

Use of the standards aids in the creation of products and services that are safe, reliable and of good quality. The standards help businesses increase productivity while minimising errors and waste. By enabling products from different markets to be directly compared, they facilitate companies in entering new markets and assist in the development of global trade on a fair basis. The standards also serve to safeguard consumers and the end-users of products and services, ensuring that certified products conform to the minimum standards set internationally.

ISO standards are principally developed by its Technical Committee (TC) framework. These are numerically sequenced from TC 1 to currently, and the latest, TC 334. Key TCs in our area of interest are:

- TC 176—Quality management and quality assurance
- TC 334—Reference materials

In addition, ISO also has a specialist committee ISO/CASCO – Conformity assessment, which is defined by its term of reference as follows.

ISO/CASCO—Terms of reference

- To study means of assessing the conformity of products, processes, services and management systems to appropriate standards or other technical specifications.
- To prepare international guides and International Standards relating to the practice of testing, inspection and certification of products, processes and services, and to the assessment of management systems, testing laboratories, inspection bodies, certification bodies, accreditation bodies, and their operation and acceptance.
- To promote mutual recognition and acceptance of national and regional conformity assessment systems, and the appropriate use of International Standards for testing, inspection, certification, assessment and related purposes.

In practice, this assigns ISO/CASCO the responsibility for the 17000 series standards; and, as we will see in later articles, an interesting discussion with respect to where the responsibility for a given standard resides within the ISO organisation.

ISO 9000

Developed by TC 176—Quality management and quality assurance, the ISO 9000 series of standards are based on seven key quality management principles (QMP).

The seven quality management principles are:

- QMP 1—Customer focus
- QMP 2—Leadership
- QMP 3—Engagement of people
- QMP 4—Process approach
- QMP 5—Improvement
- QMP 6—Evidence-based decision making
- QMP 7—Relationship management

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Principle 1—Customer focus

Organisations depend on their customers and therefore should understand current and future customer needs, should meet customer requirements and strive to exceed customer expectations.

Principle 2—Leadership

Leaders establish unity of purpose and direction of the organisation. They should create and maintain the internal environment in which people can become fully involved in achieving the organisation's objectives.

Principle 3—Engagement of people

People at all levels are the essence of an organisation and their full involvement enables their abilities to be used for the organisation's benefit.

Principle 4—Process approach

A desired result is achieved more efficiently when activities and related resources are managed as a process.

Principle 5—Improvement

Improvement of the organisation's overall performance should be a permanent objective of the organisation.

Principle 6—Evidence-based decision making

Effective decisions are based on the analysis of data and information.

Principle 7—Relationship management

Relationships management through effective communication and contract control assists the assurance of agreed outcomes from the process.

ISO 17000 series

Developed under the responsibility of ISO/CASCO, the standards under the control of ISO/CASCO, which includes this series currently consists of 41 standards related to conformity assessment.

The three key standards in our area of interest are:

- ISO/IEC 17025—General requirements for the competence of testing and calibration laboratories. This is the main ISO standard used by testing and calibration laboratories. In common with other ISO quality standards, ISO/IEC 17025 requires continual improvement. Additionally, the laboratory will be expected to keep abreast of scientific and technological advances in relevant areas.
- ISO 17034—General requirements for the competence of reference material producers. The most recent of the three, which like ISO/IEC 17025 evolved from the associated "Guide" document; the history of which will be discussed in the next article.
- ISO 17043—Conformity assessment: General requirements for proficiency testing. An essential standard used extensively in specific application areas, and which again will be discussed in future article(s).

ISO 1st Generation—the years between 1940 and 1975

The ISO organisation began in the 1920s as the International Federation of the National Standardizing Associations (ISA). It was suspended in 1942 during World War II, but after the war ISA was approached by the recently formed United Nations Standards Coordinating Committee (UNSCC) with a proposal to form a new global standards body. In October 1946, ISA and UNSCC delegates from 25 countries met in London and agreed to join forces to create the new International Organization for Standardization. The new organisation officially began operations in February 1947.

Founded on 23 February 1947, the organisation promotes Worldwide proprietary, industrial and commercial standards. It is headquartered in Geneva, Switzerland and works in 165 countries. It was one of the first organisations granted general consultative status with the United Nations Economic and Social Council.

ISO TC1, was the first Technical Committee established, and unsurprisingly, deals with screw threads and was created back in 1947.

ISO 9000 was first published in 1987 by ISO. It was based on the BS 5750 series of standards from the British Standards Institute (BSI) that were proposed to ISO in 1979. However, its history can be traced back some 20 years before that, to the publication of government procurement standards, such as the United States Department

Table 1. Key dates/timeline.

Date	Event
1920s	International Federation of the National Standardizing Associations (ISA)
1947	ISO
1947	ISO TC1
1947	Australian National Association of Testing Authorities (NATA)
1959	United States Department of Defence MIL-Q-9858
1973	TELARC—New Zealand
1979	BS 5750
1987	ISO 9000
1994	ISO 9000
1999	ISO/IEC 17025
2000	ISO 9000
2005	ISO/IEC 17025
2008	ISO 9000
2015	ISO 9000
2016	ISO 17034
2017	ISO/IEC 17025

of Defence MIL-Q-9858 standard in 1959, and the UK's Def Stan 05-21 and 05-24. Large organisations that supplied government procurement agencies often had to comply with a variety of quality assurance requirements for each contract awarded, which led the defence industry to adopt mutual recognition of NATO AQAP, MIL-Q and Def Stan standards. Eventually, industries adopted ISO 9000 instead of forcing contractors to adopt multiple and often similar requirements.

During this period, we see the first national standards being used in the Antipodean region, driven by formation of the Australian National Association of Testing Authorities (NATA) in 1947 and TELARC—New Zealand in 1973.

ISO 2nd Generation—the years 1975 to 2000

In its first released version, 9000:1987 had the same structure as the UK Standard BS 5750, with three "models" for quality management systems, the selection of which was based on the scope of activities of the organisation.

- ISO 9001:1987 Model for quality assurance in design, development, production, installation and servicing was for companies and organisations whose activities included the creation of new products.
- ISO 9002:1987 Model for quality assurance in production, installation, and servicing had basically the same material as ISO 9001 but without covering the creation of new products.
- ISO 9003:1987 Model for quality assurance in final inspection and test covered only the final inspection of finished product, with no concern for how the product was produced.

ISO 9000:1987 was also influenced by existing US and other Defence Standards ("MIL SPECS"), and so was well-suited to manufacturing. The emphasis tended to be placed on conformance with procedures rather than the overall process of management.

The global adoption of ISO 9001 may be attributable to a number of factors. In the early days, the ISO 9001 (9002 and 9003) requirements were intended to be used by procuring organisations, as the basis of contractual arrangements with their suppliers. This helped reduce the need for individual supplier evaluation by establishing basic requirements for a supplier to assure product quality. The ISO 9001 requirements could be tailored to meet specific contractual situations, depending on the complexity of product, business type (design responsibility, manufacture only, distribution, servicing etc.) and risk to the procurer. If a chosen supplier was weak on the controls of their measurement equipment (calibration), and hence QC/inspection results, that specific requirement would be invoked in the contract. The adoption of a single quality assurance requirement also leads to cost savings throughout the supply chain by reducing the administrative burden of maintaining multiple sets of quality manuals and procedures.

A few years later, the UK Government took steps to improve national competitiveness following publication of cmd 8621, and Third Party Certification of Quality Management Systems was born, under the auspices of the National Accreditation Council of Certification Bodies (NACCB), which has become the United Kingdom Accreditation Service (UKAS).

From a personal perspective, at this time I was employed by a leading company involved in the manufacture of spectrophotometric instrumentation, and who were already adopting the principles of BS 5750, this new standard (ISO 9001) introduced a new design and development control structure within the organisation, which in later years, with the advent and extensive use of control software requirements was extended to cover the testing of this essential component. This proved invaluable in later years, as described below.

1994 version

ISO 9000:1994 emphasised quality assurance via preventive actions, instead of just checking final product, and continued to require evidence of compliance with documented procedures. As with the first edition, the downside was that companies tended to implement its requirements by creating shelf-loads of procedure manuals and becoming burdened with an ISO bureaucracy. In some companies, adapting and improving processes could actually be impeded by the quality management system.

The changed requirements of this updated standard introduced, as stated above, a formal design and specification requirement on our new product development, which previously had not existed. Key specification documents now stated design, marketing and manufacturing requirements, against which products were evaluated. As stated above, this explosion of additional required documentation could have been perceived as an unnecessary burden at the time, but with the benefit of hindsight, these processes proved invaluable when the next new product in 1996 was targeted at the new and equally evolving regulated pharmaceutical market—but more of that later.

ISO/IEC 17025 was initially issued by ISO in 1999. There are many commonalities with the ISO 9000 standard, but ISO/IEC 17025 is more specific in requirements for competence and applies directly to those organisations that produce testing and calibration results and is based on somewhat more technical principles. Laboratories use ISO/IEC 17025 to implement a quality system aimed at improving their ability to produce consistently valid results. It is also the basis for accreditation from an accreditation body.

In line with the increased use of the ISO 9001 standard within our organisation, the next logical extension was for our Calibration Laboratory, which had been following ISO Guide 25 principles, to seek accreditation to the new ISO/IEC 17025 standard. This was my first experience of the dual "technical" and Quality Management requirements of this accreditation standard, but again, from a marketing/sales perspective the stated "tested once—accepted Worldwide" message being presented was seen a significant extension to the Quality message being presented by the organisation.

ISO 3rd Generation—the years 2000 to 2020

ISO 9001:2000 replaced all three former standards of 1994 issue, ISO 9001, ISO

9002 and ISO 9003. Design and development procedures were required only if a company does, in fact, engage in the creation of new products. The 2000 version sought to make a radical change in thinking by actually placing front and centre the concept of process management (the monitoring and optimisation of a company's tasks and activities, instead of just inspection of the final product). The 2000 version also demanded involvement by senior management in order to integrate quality into the business system and avoid delegation of quality functions to junior administrators. Another goal was to improve effectiveness via process performance metrics: numerical measurement of the effectiveness of tasks and activities. Expectations of continual process improvement and tracking customer satisfaction were made explicit.

ISO 9000 requirements include:

- Approve documents before distribution.
- Provide correct version of documents at points of use.
- Use your records to prove that requirements have been met.
- Develop a procedure to control your records.

2008 version

ISO 9001:2008 in essence re-narrates ISO 9001:2000. The 2008 version only introduced clarifications to the existing requirements of ISO 9001:2000 and some changes intended to improve consistency with ISO 14001:2004. There were no new requirements. For example, in ISO 9001:2008, a quality management system being upgraded just needs to be checked to see if it is following the clarifications introduced in the amended version.

ISO 9001 is supplemented directly by two other standards of the family:

- ISO 9000:2005 "Quality management systems. Fundamentals and vocabulary"
- ISO 9004:2009 "Managing for the sustained success of an organisation. A quality management approach"

Other standards, like ISO 19011 and the ISO 10000 series, may also be used for specific parts of the quality system.

2015 version

In 2012, ISO TC 176, responsible for ISO 9001 development, celebrated 25 years of implementing ISO 9001 and concluded that it was necessary to create a new Quality Management (QM) system model for the next 25 years. They subsequently commenced the official work on creating a revision of ISO 9001, starting with the new QM principles. This moment was considered by important specialists in the field as the "beginning of a new era in the development of quality management systems". As a result of the intensive work from this TC, the revised standard ISO 9001:2015 was published by ISO on 23 September 2015. The scope of the standard has not changed; however, the structure and core terms were modified to allow the standard to integrate more easily with other international management systems standards.

The new ISO 9001:2015 management system standard helps ensure that consumers get reliable, desired quality goods and services. This further increases benefits for a business.

The 2015 version is also less prescriptive than its predecessors and focuses on performance. This was achieved by combining the process approach with risk-based thinking and employing the Plan-Do-Check-Act cycle at all levels in the organisation.

Some of the key changes include:

- High-Level Structure of 10 clauses is implemented. Now all new standards released by ISO will have this high-level structure.
- Greater emphasis on building a management system suited to each organisation's particular needs.
- A requirement that those at the top of an organisation be involved and accountable, aligning quality with wider business strategy.
- Risk-based thinking throughout the standard makes the whole management system a preventive tool and encourages continuous improvement.
- Less prescriptive requirements for documentation: the organisation can now decide what documented information it needs and what format it should be in.
- Alignment with other key management system standards through the use of a common structure and core text.
- Inclusion of Knowledge Management principles.
- Quality Manual & Management representative are no longer mandatory. An organisation and its external providers (suppliers, contractors, service providers) are interdependent and a mutually beneficial relationship enhances the ability of both to create value.

ISO 9001:2015 Quality management systems—Requirements is a document of approximately 30 pages available from the national standards organisation in each country. Only ISO 9001 is directly audited against for third-party assessment purposes.

Contents of ISO 9001:2015 are as follows:

- Section 1: Scope
- Section 2: Normative references
- Section 3: Terms and definitions
- Section 4: Context of the organisation
- Section 5: Leadership
- Section 6: Planning
- Section 7: Support
- Section 8: Operation
- Section 9: Performance evaluation
- Section 10: Continual Improvement

Essentially, the layout of the standard is similar to the previous ISO 9001:2008 standard in that it follows the Plan-Do-Check-Act cycle in a process-based approach but now further encourages this to have risk-based thinking (section 0.3.3 of the introduction). The purpose of the quality objectives is to determine the conformity of the requirements (customers and organisations), facilitate effective deployment and improve the QM system.

Before the certification body can issue or renew a certificate, the auditor must be satisfied that the company being assessed has implemented the requirements of sections 4 to 10. Sections 1 to 3 are not directly audited against, but because they provide context and definitions for the rest of the standard, not that

of the organisation, their contents must be taken into account.

The standard no longer specifies that the organisation shall issue and maintain documented procedures, but ISO 9001:2015 requires the organisation to document any other procedures required for its effective operation. The standard also requires the organisation to issue and communicate a documented quality policy, a QM system scope and quality objectives. The standard no longer requires compliant organisations to issue a formal Quality Manual. The standard does require retention of numerous records, as specified throughout the standard. New for the 2015 release is a requirement for an organisation to assess risks and opportunities (section 6.1) and to determine internal and external issues relevant to its purpose and strategic direction (section 4.1). The organisation must demonstrate how the standard's requirements are being met, while the external auditor's role is to determine the QM system's effectiveness. More detailed interpretation and implementation examples are often sought by organisations seeking more information in what a very technical area can be.

In 2000, I moved to a new manufacturing organisation, where although the products were in many cases significantly different to my previous employment, the ISO 9001 standard still provided the essential QM system to ensure a "Quality" product. This new organisation also had a Calibration Laboratory, supplying product to a multitude of industries, including pharmaceutical quality assurance (QA) laboratories, and accreditation of this laboratory to these new ISO 17000 standards has been a principal task—but more of that later.

ISO/IEC 17025—There have been three releases; in 1999, 2005 and 2017.

The most significant changes between the 1999 and 2005 release were a greater emphasis on the responsibilities of senior management, explicit requirements for continual improvement of the management system itself, and communication with the customer. It also aligned more closely with the 2000 version of ISO 9001.

The 2005 version of the standard comprises five elements: Normative References, Terms and Definitions, Management Requirements, and Technical Requirements. Management requirements are primarily related to the operation and effectiveness of the QM system within the laboratory. Technical requirements include factors that determine the correctness and reliability of the tests and calibrations performed in the laboratory.

The 2017 version of ISO/IEC 17025 has modified this structure to be Scope, Normative References, Terms and Definitions, General Requirements, Structural Requirements, Resource Requirements, Process Requirements, and Management System Requirements. General Requirements and Structural Requirements are related to the organisation of the laboratory itself. Resource Requirements cite those issues related to the people, plant and other organisations used by the laboratory to produce its technically valid results. Process Requirements are the heart of this version of the standard in describing the activities to ensure that results are based on accepted science and aimed at technical validity. Management System Requirements are those steps taken by the organisation to give itself QM system tools to support the work of its people in the production of technically valid results.

The initial version of ISO 17034 was published in 2016, superseding the associated ISO Guide 34.

The personal journey through this evolution will be discussed more fully in the next article.

ISO 4th Generation—from 2021 forward

The ISO 9000 standard is continually being revised by standing TCs and advisory groups, who receive feedback from those professionals who are implementing the standard. Therefore, this standard will continue to evolve, but from a personal perspective, I would suggest that it has now come of age and now forms one of the fundamental "Pillars of Quality" detailing the QM system.

> *"…Quality is a perceptual, conditional, and somewhat subjective attribute and may be understood differently by different people…"*

This statement underpins the contractual considerations clearly defined in the ISO 9001 quality standard as described in this article.

Recently updated, or published, ISO/IEC 17025:2017 and ISO 17034:2016 currently reflect the "state of the art" with respect to these standards and are, therefore, unlikely to be revised in the near future. However, like their ISO 9001 counterpart, the ISO TCs associated with these standards will continue to review and develop these standards, and again this evolution will be discussed in future articles.

So, we now have in place a fully developed and established QM system, supported by the ISO 9000 standard, internationally by ISO, and used Worldwide.

The next article in the series will explain how this QMS underpins the associated 17000 series standards and the organisations that use them.

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SAMPLING COLUMN

WHAT are sampling errors—and WHAT can we do about them? Part 2: Sampling and weighing—different, but the same...

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This cannot be true—surely sampling and weighing are *different* activities. Well yes—and no! Sampling and weighing of traded metal, mineral and agro commodities are different activities—but at one or several stages in the supply chain they will come together in a single focus point, which is value ($, EUR). The commercial value of bulk commodities depends on two factors, quality and quantity. As an example, a shipment of iron ore with a certain certified weight cannot be traded without a reliable declaration of its quality, iron percentage. Similarly, a shipment of rice (assuming pure rice with no contaminants) cannot be paid for without its certified weight. At least once in all supply chains, someone in treasury will look at the final output of what has to be *assumed* is the result of diligent representative sampling and reliable weighing. But the final accounting will not show the overall accuracy and precision of sampling, preparation and analysis, and neither show the accuracy class of the weighing device. In the final accounting, this will all be the same for the user: what is important is the monetary value that is to be paid or received. The demands for minimisation of both sampling and mass determination errors are often hidden, but absolutely critical. This column specifically focuses on weighing errors in more detail, adding essential theoretical elements and practical know-how to the framework of the Theory of Sampling.

Quality and quantity—equal factors

In the world of commercial sampling of commodities this is nothing new. Historically, this was one of the driving forces why Pierre Gy started to address the fundamental conceptual and theoretical issues and the critical practical problems in *sampling*. Gy started to investigate the quality issue in earnest in his first assignment in 1946 in the then Belgian Congo, when he started out working as a research engineer for the mining and processing trade organisation Minerais et Metaux.[1–3]

Gy realised that sampling of bulk particulate materials is a challenging combination of understanding the concept of heterogeneity and mastering the appropriate engineering principles involved, which many at the outset would believe could be significantly helped by *statistics*. After all, the term *sampling* is for very many (individuals, organisations, academic disciplines etc.) a statistical term. However, it turned out that statistics, based on analytical results, by itself would not deliver the solution to how to optimise sampling procedures and equipment when facing heterogeneous materials. Gy's monumental theoretical analysis, developed over the next 25 years revealed the need for a set of *sampling errors* which are not all of the traditional statistical type, systematic vs random errors. In particular, Gy's analysis uncovered *bias-generating errors* caused by the interaction of material

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heterogeneity and ill-reflected sampling procedures that had to be dealt with in a more comprehensive manner.[4,5] But statistics does play a role in the Theory of Sampling (TOS), which manifests itself in the fact that numerical determination of the quality factor is an *estimation*, an estimation of the composition of a lot.[6]

But what about determination of the *quantity* of a lot, i.e. the *weight* of a lot? This is the subject matter covered in this column.

Representativity—at the centre of everything

A critical issue is: what are the *criteria* that need to be satisfied for a compositional estimation to be declared "representative"? Is it enough that certain error tolerances of the quality and quantity of an analytical aliquot are suitable for the needs of the person that will use it; for contractual purposes, for example? There is a practical side to this issue as well, one that has prompted introduction of the term "fit-for-purpose representativity".

With the TOS as a guiding framework,[6–8] it turns out that these issues are rather intertwined, but fully resolvable. Assuming that the specific analytical method used can be relied upon to be "in statistical control", i.e. the analytical process is accurate and precise according to universally agreed upon characteristics, a condition well complied with by all the world's scientific, technical and commercial analytical laboratories. Then, in order for the analytical determination to be representative, it is necessary-and-sufficient that both the analytical aliquot, as well as the previous multi-stage samples and sub-samples, are **all** representative of the primary lot material.[4,5]

This understanding is one of the TOS' greatest achievements, that the entire "from-lot-to-aliquot" pathway is causally connected to the analytical determination and whether analytical results can correctly be considered representative, or **not**. In fact, the TOS stipulates that there is no characteristic of a sample itself that can vouch for its status—**only** the status of the entire *sampling pathway* is able to pass judgement on whether the test portion is representative or not. Thus, in a very direct sense, analytical results *depend* on the full "lot-to-aliquot" pathway—which *can* be representative but certainly also **not**, *ibid*. It matters very much that managers of analytical laboratories and Testing, Inspection, Certification (TIC) companies are aware of this critical connection; this context is described in depth in References 9 and 10.

However, at this point we *may* have already lost the interest and attention of the treasury department.

Treasury: *"Estimation? … Error tolerances? … Representativity? So what? The monetary value on the invoice is **all** that matters and the commodity will not change because of all that."*

How correct—and how wrong at the same time!

Money rules the world—it is often claimed

The commodity does indeed **not** change in and of itself (loss, theft or damage excluded), but **what if** the analytical sample was not representative of the original lot, which it is always tacitly *assumed* to represent *without ambiguity*? This is the *raison d'etre* for the TOS.

If so, the invoice value *will* actually vary and be different if the commodity is sampled and tested at two or more TIC locations, e.g. loading port vs discharge port, or similar scenarios: lab 1 vs lab 2; buyer vs seller. Why? Because lot materials are always heterogeneous, a sampling bias will always ensue if all sampling operations involved in TIC are not representative. Thus, based on the TOS' 70+ years' experience, without guarantee for representativity, analysis of heterogeneous lots at two locations will assuredly always lead to *dissimilar* analytical results … and this ambiguity will only proliferate were additional attempts tried with the purpose of checking whether the sampling bias is constant. However, according to the TOS this can never be.[5,6]

This is the point where we are absolutely sure to lose the treasury department:

Treasury: *"The same lot, characterised at two ports, will **always** give rise to dissimilar analytical results? Always?" The treasury department, and/or the trader (commodity trader), will now likely hedge: "OK then, yes sure, this **may** be so, but we have the appropriate technical staff to take care of all this sampling".*

However, what about weighing—in what sense can this be "the same as sampling"?

Sampling vs weighing

Well, weighing is also an act of estimation when weighing is carried out on an industrial scale as, for example, with traded bulk commodities. The question for weighing is, *as with sampling*: how representative shall it be? How *accurate* shall the mass determination have to be? Ultimately, within the weighing domain there are in fact both *incorrect* and *correct* weighing errors, in perfect analogy to the domain of sampling! To be demonstrated below.

Sampling errors: a breakthrough concept

Pierre Gy was able to come to grips with the reasons for non-representative sampling; there are several reasons.[4,7] He identified and analysed in detail the consequences of both unmitigated *Incorrect* Sampling Errors (ISE) and *Correct* Sampling Errors (CSE). The ISEs are:

- Incorrect Delimitation Error (IDE)
- Incorrect Extraction Error (IEE)
- Incorrect Preparation Error (IPE)
- Incorrect Weighting Error (IWE)

ISEs are responsible for creating a sampling bias, which must be avoided at all costs.[11] Below, we exemplify all these types of ISE in the weighing domain.

Weighing Incorrect Delineation Error (wIDE)

In sampling, avoiding IDE is all about strict reproducibility in delineating incremental cuts in a correct fashion, e.g. being able to take a full core from top to bottom in a stockpile (**all** the way to the bottom), or taking a complete plane-parallel cross-section across the full material stream on a moving, or stopped, conveyor belt.

In weighing there are similarities when it comes to correctly delineating the mass that is weighed.

SAMPLING COLUMN

Figure 1. Falling stream cutter with contorted edges that result in incorrect delineation (IDE).

An example from the weighing domain would be a weighing device that gradually moves away from its calibration condition: measurement "drift". This is often the largest attributor to a weighing bias. If not properly trained, the operator of the weighing device is often not aware of this, but strongly believes that it is sufficient just to observe the service interval between calibrations prescribed in the manual accompanying the acquisition of the device. With industrial weighing devices, such as belt-scale weighers, there are many variables that each will have an impact on the device drifting further and further away from its last state of validation.

The analogy in the sampling domain is like not being able to observe the development of the crooked and contorted edges of a cross-stream sample cutter, Figure 1. In both cases a non-constant IDE is gradually developing, but this non-constant bias is hidden from view.

The following is a list of salient IDEs associated with a belt-scale weigher (Figure 2):

- Change in belt length: because the physical belt material stretches over time
- Change in belt tension: because of neglected checks and service of tensioners
- Change in drum diameters: because of poor cleaning causing dirt between drum and belt
- Mis-aligned weighing idlers: because of slacking of the belt
- Slipping and/or dirt coverings of the speed sensor

Weighing IDEs must be eliminated to avoid bias, exactly as in the sampling domain. This is fully possible through frequent, or continuous, inspection and diligent maintenance of the mechanical weighing system, which would be proper diligence, more conscientious than just referring to the calibration validity sticker—if there is such a thing in the first place! It is all about inspection and maintenance here, about frequent checks and verifications. Above all, it is about proper training of the personnel involved—and not only about weighing, the full TOS framework needs to be in mind.

Calibration: operation that, under specified conditions, establishes a relation between the quantity values with measurement uncertainties (provided by other/known measurement standards and corresponding indications with their known measurement uncertainties).
Verification: provision of objective evidence that a given item fulfils the specified requirements.

Weighing Incorrect Extraction Error (wIEE)

In the sampling domain, one is committing an IEE if not all of the (correctly) delimited cut is actually extracted. In the weighing domain this means that not all material is weighed even though it has been correctly delimited.

It is instructive to perform a "thought experiment" for weighing trucks over a weighbridge (Figure 3). Of course, interest is not in the mass of the trucks themselves, but specifically only in the mass of the cargos. For correct "extraction" of the mass, i.e. the correct determination of the weight, the requirement is, therefore, to weigh the truck twice: full and empty. The delimited difference between those two weighing results constitutes the cargo mass.

The weighing IEE, wIEE, crops up as a consequence of an attempted logistical shortcut during practical *cycling* of loading or discharge operations in a port, where the same trucks are used to

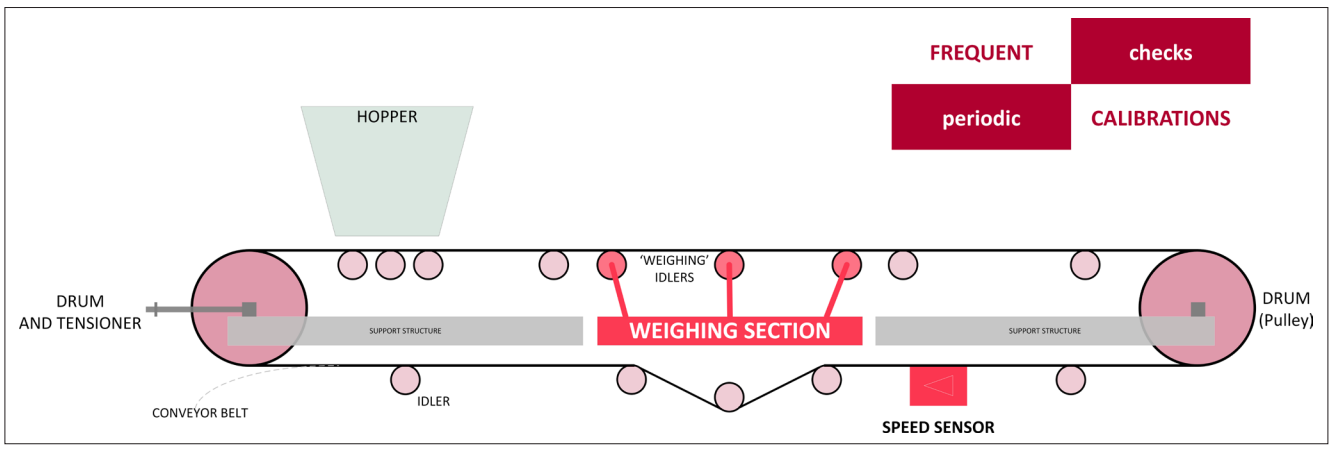

Figure 2. Principal set-up and key parts of a belt-scale weighing device.

transport a commodity over a relatively short distance. The wIEE originates here with the unfounded assumption that the mass of a specific empty truck is *constant* within a bracketed time frame and a within a well-defined specific port footprint. But it is not unheard of that the "burden" of weighing is reduced by only passing laden trucks over the scale and using the empty truck mass for more than one "trip" from storage to weighbridge to quayside and vice versa… or rather **not** vice versa, but proceeding straightaway to loading again. This means weighing any "unextracted" cargo remnant mass twice over, for example all of the two tons as seen in Figure 4 (right panel). The value of two tons of this specific material corresponds to EUR 2500; a shipment may consist of ~400 truckloads. One may imagine this to happen, say for every every fifth truck—with the result of EUR 200,000 worth of weighing error. The point here is also that this type of wIEE may not necessarily occur with any regularity with obvious consequences.

So far, the above "two out of two" signifies that certain ISE have direct counterparts in the weighing domain (IDE, wIDE; IEE, wIEE).

What about IPE (or IWE)?

The IPE, however, is an issue where there is no easy comparison, simply because there is not much to "*prepare*" in the weighing domain—and drawing a parallel with electric current fluctuations and its impact on the load cell signal and its calibrated value in kilograms may be more than a bit farfetched.

But there are occasions in which a critical but sometimes unrecognised IPE in the sampling domain, evaporation of **moisture** (loss of moisture), *may* have an analogue in the weighing domain. In both domains this takes the form of unrecognised, uncontrolled or unmitigated loss of moisture which is actually determined as *weight differences*. The classic example is a primary wet sample having to comply with a logistical waiting period in a dry environment before being transported to the central laboratory—but left in a container without a waterproof lid in high ambient temperatures. This scenario depicts unrecognised moisture loss that will interfere with subsequent moisture determination, which structurally will always be too low by an unknown proportion. This clearly leads to an inconstant, significant sampling bias (N.B. there are also other "agents" at work in the IPE domain; the above is not a comprehensive treatment.)

Moisture is a key parameter in most commodity trade TIC protocols, where similar mishaps may occur if sufficient professional competence is lacking. Perhaps the easiest way to cover all such possibilities is to focus on the *time intervals* in question, i.e. the *time duration* in which wet samples may unwittingly lose moisture, partially or completely. A disconnect between time and place of sampling and time and place of weighing is clearly a sampling error.[a] As a graphic example: what is the meaning of weighing a commodity of gold concentrates, packed in big bags, at the time when the consignment is loaded into the cargo

Figure 3. Full (container doors closed) container on truck: gross mass. After discharge, the empty container (doors open), the truck is weighed again: tare mass. The difference will be the cargo mass.

Figure 4. Left: Trucks moving in a port area from storage, via a weighbridge to quayside for discharge (v.v.). Right: Truck tipping cargo at quay for loading onto a receiving vessel. Inside the yellow circle 2000 kg of cargo remnants are visible that will remain inside the truck during its next trip (wIEE).

[a]There is a close connection to the topic "error" vs "uncertainty" presented and discussed in the preceding column,[12] in which can also be found an example of a strict parallel w.r.t. a mismatch error (disconnect) between the acquisition locations of spectra and reference samples [X,y] in a multivariate calibration data analytical context.

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holds of a container ship … when this is in fact ten days (10) **after** the "freshly filter-pressed concentrate" was sampled (following all the necessary principles in the TOS) during filling of the bags at the refinery plant. Unavoidably, *some* moisture will have seeped out of the bags in the 10-day interval prior to weighing, but how much? And was the moisture loss of similar magnitude for all bags? The mass of this moisture obviously should have been weighed at the same time as—and thus complementing—the compositional sampling! *Somebody*, or *some protocol*, is manifestly responsible—hence we are dealing with a sampling error, in this case a logistical error, an error that *could* and *should* have been avoided. Whether this scenario should be considered as a "classic" IPE or as a weighing IEE (wIEE) does not really matter. Either way, it is of critical importance to be in command of enough TOS and practical weighing competence to understand the manifest need to **eliminate** such an error, as no type of subsequent correction is ever possible.

ISE: Weighting

This topic may appear a little complex: please pay close attention to the letter "**t**" as what follows is about a technical weigh-**t**-ing error in weighing. Again, use is made of a belt-scale weigher as an example, not because they are flawed by design, but because they are very often used incorrectly—and they make for a particularly clear demonstration.

Figure 5 shows what is happening when mass is supposed to be determined by *weighing*, but without considerations of potential pitfalls. For an accurate mass determination to be possible, there must be a certain *minimum load* on the belt-scale weigher. If not, the tension of the (mostly) empty belt will prevent the downward force exerted by the "spotty" material stream on the belt to be registered by the load cell(s) in the weighing section. It is, therefore, important that the on-belt loading rate during cargo handling operations is properly controlled at all times, also during start-up and close to termination. On-belt loading rates should be *constant* as much as practicalities allow, so as to result in a *steady state* on-belt material steam (constant material flux). Operators of front-end-loaders that pile cargo onto the belt, crane operators that grab cargo from the holds of a vessel *should* be properly trained and well aware of this pertinent minimum load requirements of the weighing device. For professional work, it is unacceptable to let cargo "trickle" onto the belt for long(er) periods of time as the mass(es) involved will be *underrepresented*. Its proper mass(es) will go unnoticed. This is clearly a technical weigh-**t**-ing error—which unavoidably creates a weighing bias to be avoided "at all costs". *Somebody* will clearly have to pay for the un-weighed mass(es), but whether this is the buyer or the seller is equally unacceptable from a professional TIC point of view. The responsibility of the TIC certification mandate is to eliminate this kind of unnecessary wISE.

Correct Weighing Errors …

Treasury: *Sorry, what? "Correct … Errors, how can an error be correct?".*

The reader is referred to Gy's original definitions of correct vs incorrect errors.[5,10] In the sampling domain, CSEs can never be completely avoided as they are a function of the interaction between the quality variation of a heterogeneous lot and the sampling process with which increments are selected and extracted in practice. Any estimated sample composition, and hence also of the estimated lot composition, will inevitably show a difference with respect to the *true* lot value.[1–6,11] The magnitude of this CSE (most often it is the sum of the Fundamental Sampling Error and a residual Grouping and Segmentation Error) needs to be *managed* by first setting an acceptable CSE target threshold and then designing a sampling plan in which the number of primary increments (*Q*) is the key parameter with which to make the total CSE in compliance—for significantly heterogeneous materials, more TOS facilities may also have to be used. This is where the full TOS framework must be at the disposition of the operator, supervisor, CTO …

But in most weighing scenarios of *bulk commodities*, the whole cargo must be weighed. The situation here often is that what the properly managed, meticulously calibrated and well-maintained weighing instrument shows… is the **true** weight. But this is based on a **wrong** assumption, as will be explained.

ISO standards, such as ISO 12743, provide examples of overall targets for desired CSE magnitudes. Remember that

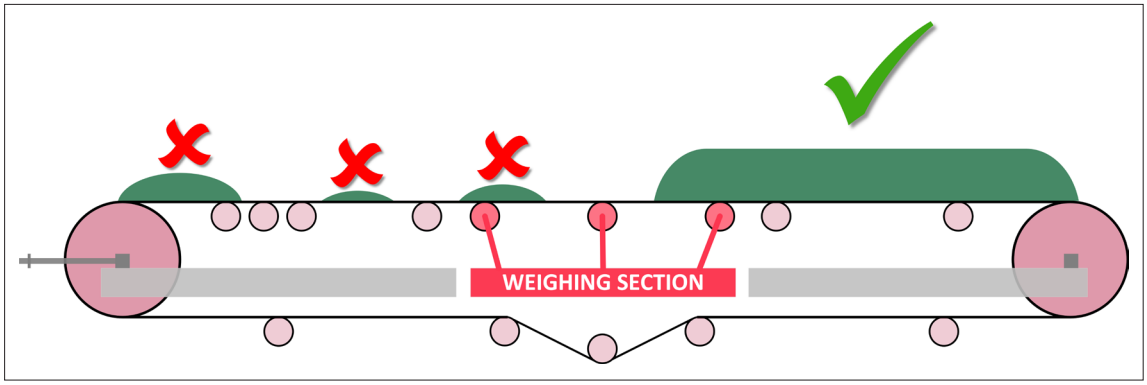

Figure 5. Left (with error marks): Incorrect loading of the belt resulting in too low weight signal. Right (with correct check-mark): Correct, uninterrupted loading of the belt resulting in weight signal as designed.

For determination of cargo mass there are sometimes occasions where a standard *statistical sampling* is required, for example regarding weighing shipments of bagged rice where a certain number of these bags are the only ones actually weighed. The corresponding average result is then multiplied by the tally of the whole number of bags in the bag population. Most sampling and weighing operations are relatively "easy" for commodities showing up in this manner of conveniently *bagged* volumes/masses.

at this stage it is traditionally *assumed* that all bias-generating errors (ISE) have indeed been eliminated (a very convenient assumption). But, assumptions are not always right….

Food for thought: A target value for standard deviation of nickel determination may be, say, 0.2% (absolute). With precision at 95% confidence, roughly twice standard deviation gives us a target of 0.4%, IF all incorrect errors have indeed been removed, all that remains **is** precision only. Weighing Standards such as issued by OIML[b] and NIST[c] are manifestly based on this fundamental assumption that there is no bias. Confusingly, however, these weighing reference standards still speak of "accuracy class" and not "precision class". "Accuracy classes" are decided upon according to the number and the value of scale divisions of the pertinent weighing devices. This means that the accuracy of a scale is dependent on a value expressed in a unit of measurement (e.g. kilogram) between two consecutive division indications. Let's again take the weighbridge as an example: most weighbridges are of OIML or NIST accuracy Class III, which means they have between 500 and 10,000 scale divisions. So, for a Class III weighbridge of 50,000 kg capacity and 500 scale divisions, the smallest unit indication is 100 kg. For another Class III weighbridge of 50,000 kg capacity but 10,000 scale divisions, the similar unit indication is 5 kg. It is very clearly **not** accuracy that is discussed here, but *precision*—QED.

Augmented TOS insight: The number of scale divisions in the weighing domain **is** what the number of primary increments is in the sampling domain! The higher the number of scale divisions, the more precise the weighing will be. It will perhaps not come as a surprise that the price of a weighing instrument shows a clear correlation with the number of scale divisions it provides. This situation prompts some wondering at the all-important treasury department…

"Wow", so the inexpensive, yet contractually binding Class III weighbridge at our receiver port in Houston, TX, can have a 20 times greater error than my own expensive weighbridge in Rotterdam with its "superior" 10,000 scale divisions?" Well yes, but this is not all… The precision target for Class III weighing devices may be about more than just scale division. The Maximum Permissible Error (MPE)[d] for Class III weighing devices according to OIML can be three (3) scale divisions; while for NIST Class III it can be up to five (5)!

Treasury: *"What? So my container that was weighed as 39,500 kg may have had a MPE of 60 kg here in the Netherlands, but our recent dispute, where the container was weighed for payment in the USA as 39,000 kg,* ***could*** *just have been a result of the MPE of 500 kg 'over there'?"*

Well yes, but wait, there is still more! Remember that for proper determination of cargo mass, one actually needs to weigh the container **twice**: as full and as (assured) empty. Consequently, one will then need to consider MPE **twice**…. Keep your weighing balance sheet flexible!

All this potential confusion (if you are not a very experienced, indeed a chartered operator) is all for scales that has the same accuracy class on their treasured calibration certificate, but which in reality are not identical in practice. And the present initiation to the weighing domain has not even looked at different types of weighing instruments and different accuracy classes yet!

Minnitt hit the nail on its head when he stated:[13] "The costs of sampling installations and new equipment are usually hard for management to accept because the adverse effects of poor sampling practice never appear on the balance sheet. The mining industry is replete with stories about the adverse effects of trying to save money on sampling equipment and installations."

To which the present authors would like to add: "Sampling and weighing are the same type of criticality for more fully transparent balance sheet and final report information".

$MPE_{weighing}$ is a Correct Weighing Error and should be given the same attention as a Correct Sampling Error!

Weighing along the mine-to-loading port-to-cargo-to-discharge port-to-balance sheet

Here is a way to try to express the cost of weighing imprecision as a result of different devices available at the principal locations along the commercial TIC pathway. It is a thought experiment of weighing a commodity along the full supply chain from mine to terminals and ports to its destination. For this demonstration we make use of a commodity parcel which is prescribed a precise weight of 5000 tons—it is not the weight *per se* that is of interest, it is the *deviations* from this nominal weight it experiences on its merry way. This parcel is, furthermore, completely oblivious to changes in moisture a.o.—not a gram of moisture was lost

[b]Organisation Internationale de Métrologie Légale/International Organization of Legal Metrology

[c]National Institute of Standards and Technology, USA

[d]For readers not in full TOS command, apologies for a slight possible confusion here, as MPE is also known as the acronym for Minimum Possible Error. However, from the specific context there is never any serious misunderstanding possible; the latter MPE applies to variographic analysis, while the former MPE pertains to weighing exclusively; if necessary the terms $MPE_{variographics}$ vs $MPE_{weighing}$ can be used.

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Methods of Weighing, Standards, Typical details and Errors for Non-Ferrous shipments							
Type of Mass Determination	Standard	OIML		NIST		ISO 12745	
		Accuracy Class	MPE	Accuracy Class	MPE	Min. C_v	Max. C_v
Draft survey	United Nations ECE Draught Survey Code	–	–	–	–	0.5%	2.5%
Barge survey	API Manual Chapter 17 Section 14	–	–	–	–	0.5%	2.0%
Conveyor belt	OIML R050 / NIST Handbook 44 - 2.21	0.2 0.5 1 2	0.2% 0.5% 1.0% 2.0%	–	0.5%	0.4%	>3.5%
Weighbridges	OIML R076 / NIST Handbook 44 - 2.20	III	±5 e	III or III L	≥5 e	0.1%*	0.5%*
Hopper scales (totalising)	OIML R107 / NIST Handbook 44 - 2.22	0.2 0.5 1 2	0.2% 0.5% 1.0% 2.0%	III or III L	±4 e	0.1%*	0.25%*
Crane scales (totalising)	OIML R107 / NIST Handbook 44 - 2.22	0.5 1 2	0.5% 1.0% 2.0%	III or III L	≥4 e	0.15%*	0.4%*
Platform scales	OIML R076 / NIST Handbook 44 - 2.20	III	±3 e	III	±3 e	0.05%*	0.2%*

*at gross loads the variance for the net wet mass of a single transportation unit is equal to the sum of the variances at gross and tare loads

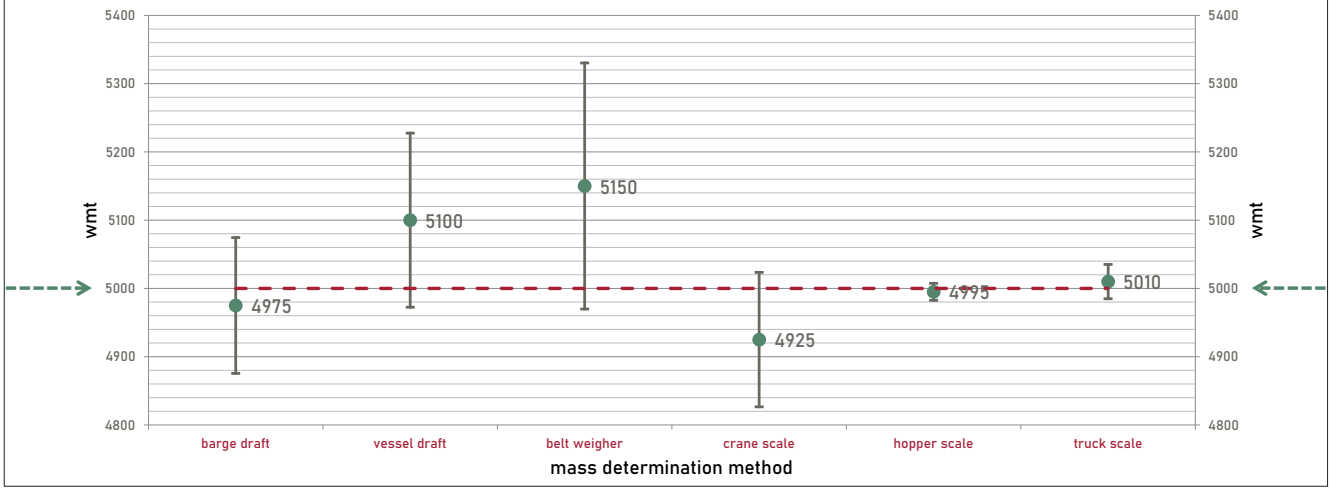

Figure 6. Top: Table with methods of weighing and interpretation of precision (MPE and Coefficient of variation). Bottom graph: Visual representation of mass estimations and precision "whiskers" of different weighing methods on the same nominal 5000 tons cargo.

in transit, and not a kilo was picked up as dirt (no IPE). But the commodity was weighed with the different devices and methods in use at the principal locations shown in Figure 6, each with their own precision characteristics. The magnitude of imprecision is expressed by the length of the whiskers extending from each estimated mass (±2std).

Each weighing method estimated the mass of the commodity according to appropriate manuals and standards, and importantly, MPE was **not** exceeded anywhere. Yet the maximum difference between six weighing methods, all used appropriately and in full compliance, was no less than 225 metric tons. This is an example slightly on the extreme side, but fully realistic. In this context, using the same commodity as in the wIEE example above (EUR 1250/ton), *some trading entity* would have unnecessarily lost or gained the equivalent of EUR 280,000 depending on which weight estimate was used. Far from trivial in commodity trading… and great for the present didactic demonstration.

The lesson is clear: there is sampling expertise (**use it well**), and there is weighing experience (**use it well**)—and your TIC partner better be fully competent in **both aspects**. Sampling and weighing are two sides of the same TIC coin.

Sampling and weighing—different but the same…

Based on Reference 14: "From the early conceptual stages of designing logistics of a port or terminal where sampling and weighing is needed, all the way to manual sampling for lack of other options, expert advice should always be taken to ensure that:

- Proper unrestricted 'access' is available for correct sampling equipment [the TOS' Fundamental Sampling Principle must be complied with, at all times and at all locations].
- Sample mass and frequency are 'selected' in accordance with the specific heterogeneity characteristics of the material vs the desired risk for being wrong.
- Sampling increments, or cuts, are taken by a properly designed and maintained plan that assuredly will 'include' all particles of the lot

without changing the commercial characteristics in any of the subsequent processes leading to the final portion that is tested."

The parallel with weighing:

- There is a proper location and an appropriate instrument for correct weighing.
- Accuracy class and scale divisions are "selected" in accordance with the specific material properties—**price**!—vs the desired risk for being wrong.
- Weighing follows a properly designed and maintained plan that will ensure that all particles of the lot will be weighed; nothing is added, nothing is lost.

Conclusions

This column only offers an *initiation* to the domain of weighing as a critical complement to the sampling domain; this column presents critical elements for an augmented TOS framework.

It would appear that in the *weighing domain* most attention is given to the technology involved, i.e. to weighing devices and their installation, and to calibrating and verification (most likely carried out during commissioning), while often neglecting their true design objectives and especially the actual performance during long(er) lifetimes in action where "better-safe-than-sorry" checks and inspection are of critical importance. Compare with the *sampling domain*, where focus all too often is overly on analysis *s.s.* and very often focused on Measurement Uncertainty ($MU_{analysis}$), to the neglect of the full complement of possible sampling and sub-sampling errors that manifestly all reside in the *before analysis domain*.

Typical *weighing domain errors* (wIDE, wIEE, $MPE_{weighing}$) were introduced and illustrated with the intent to augment the TOS' framework. The TOS is the only guarantee for sampling representativity due to bias that *could* have been avoided and precision that *could* have been achieved. The analogue scenario in the weighing domain concerns an unnecessary loss of trust w.r.t. certified weight declarations.

Since (in the context of the present discussion) "value" = *representative* "composition" × *unbiased* "mass", sampling and weighing are both different, and the same… Thus, the final outcome of sampling and weighing marry each other and merge into the same commercial unit of measurement: **value**, Figure 7.

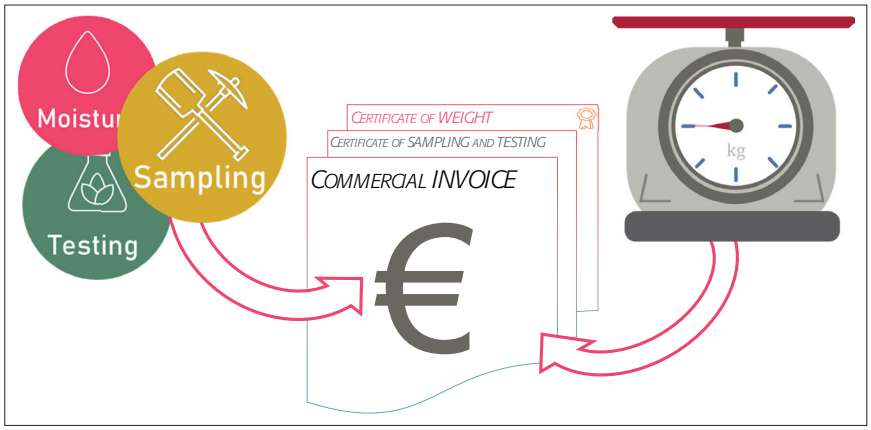

Figure 7. Sampling and weighing ultimately merge into one value: the one on the invoice.

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SAMPLING COLUMN

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Cleaner in the lab

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My lab was the central lab in a suite of three adjacent labs, which were essentially rectangular, and divided by glass windows along the dividing walls. These windows essentially went from bench-top to ceiling and, as one would expect, periodically required cleaning. These labs were before the days of the current Health and Safety regulations, and, therefore, due to the readily available bottles of 0.880 ammonia and concentrated hydrochloric acid in the lab, surfaces were liberally coated with white ammonium chloride.

Our DU was located on one of these side benches, and on the day in question, the operative from the cleaning company had been tasked with cleaning the aforesaid windows. He was an individual we had not seen before and duly arrived with his bucket and tools, and started to clean the glass window in the lab door.

At this point, and with the manager out of the lab, without asking anybody he duly picked up his bucket, and climbed onto the lab bench, and before anybody could say anything started to clean the windows, but worse was yet to come—because he couldn't easily reach the top, so he stood on the "black box" on the bench to allow him to reach the top!

At this moment the lab manager returned, and literally "hit the roof", ...you can guess the rest?

However, if you've even seen a DU—the case is essentially a rigid box section—you may not be surprised that the DU still worked perfectly after this episode!

John Hammond is an experienced analytical scientist, spectroscopist and technical marketing professional, skilled in the development, production and marketing of key analytical instrumental concepts and product into highly regulated and controlled industries. A Fellow of the Royal Society of Chemistry (FRSC), executive Working Group convenor of ISO/TC334 and an Expert Advisor to the United States Pharmacopeia, General Chapters, Chemical Analysis committee.
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The Beckman DU spectrophotometer. Photo courtesy of the Beckman Institute for Advanced Science and Technology at the University of Illinois Urbana-Champaign

APPLICATIONS

QA/QC in beverage production: cocoa mix and powdered drinks

To achieve good solubility, the particulates contained in powdered beverages are most often engineered to be very fine. Thus, visual examination or a conventional macroscopic analysis usually cannot or only partially provide the necessary information about the product. Advanced analytical methods are required to accurately analyse the composition of powdered beverages. FT-IR imaging enables identification of foreign contaminants as well as the individual major ingredients in a mixture by creating a chemical map to visualise the overall distribution.

Bruker Optik

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NH_3 detection overview

Detection of low levels of NH_3 in H_2O rich gas streams is important in a number of application areas such as refrigeration, chemical industry, automotive and energy production. When analysing NH_3 in H_2O gas streams the major problem with detection of low levels of NH_3 occurs because of the spectral overlap between the *m/z* 17 of both water and NH_3.

Hiden Analytical

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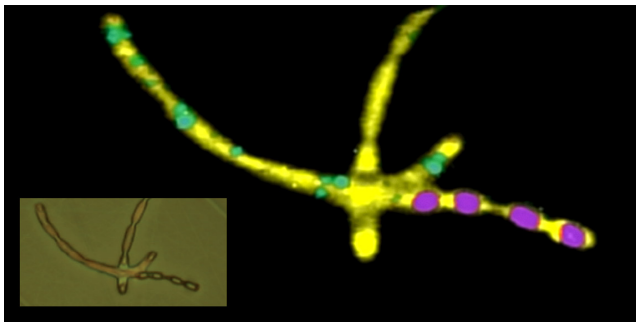

Raman imaging and correlative techniques in life sciences

Confocal Raman imaging is well suited for the study of living cells in their physiological surroundings as it is a non-destructive, label-free chemical characterisation technique. Combined with other techniques such a fluorescence microscopy or scanning electron microscopy, Raman imaging can deliver a more comprehensive understanding of a sample. Recent studies have shown that Raman microscopy can even be used to discriminate between malignant and healthy cells. This application note describes how Raman microscopy, alone or in combination, can investigate plant cell walls, macrophages and bacteria, and recognise atherosclerosis, differentiate malignant cells and monitor lipid uptake among other capabilities.

WITec

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Rapid plastic ID with extended range Raman

Identification of plastic types for separation is key to effective recycling, and Raman spectroscopy offers the speed and specificity to help. In this application note, the WP 785 ER extended range Raman spectrometer is introduced as a tool to discriminate between plastic types, due to its spectral range well beyond the fingerprint region, its high sensitivity and signal-to-noise ratio (SNR), and excellent reproducibility. It shows the ability of this extended range Raman spectrometer to identify the chemical nature of plastic items down to the exact variety within some of the more diverse polymer families, and the presence of additives.

Wasatch Photonics

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Advantages of volume phase holographic gratings

The term "grating" or "diffraction grating" often brings to mind a surface relief grating, with ruled lines and a delicate surface. Working in transmission, however, can open up many new options for the optical designer. In this tech note, we consider one special type: volume phase holographic (VPH) gratings. With benefits ranging from superior optical performance and design flexibility to robustness and consistency, VPH gratings are ideal for applications like laser pulse compression, spectroscopy, optical coherence tomography and astronomy.

Wasatch Photonics

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ATOMIC

New optical emission spectrometer

Hitachi High-Tech Analytical Science has expanded its metals analysis range with the OE720 optical emission spectrometer, which has the same performance as the OE750 but offers a price advantage for those who do not need additional gas analysis capability. The OE720 covers the entire spectrum of elements in metal except for gases like oxygen and hydrogen. Hitachi OE series instruments use their LightWing optic design, coupled with CMOS detector technology. This combination achieves the wide wavelength range necessary to measure the entire range of elements within metals at ppm levels. LightWing optics also reduce argon and power consumption, thanks to their ultra-compact design, and have a fast start-up and measurement time. The OE720 is suitable for aluminium casting, as it can determine phosphorous to very low limits in near eutectic and hypereutectic aluminium–silicon alloys. It can analyse antimony, bismuth, lithium, strontium and sodium, and tramp and trace elements, ensuring these can be controlled within the aluminium melt for optimal structural modification. This aids high throughput production, where the quality of the melt needs to be verified at several points.

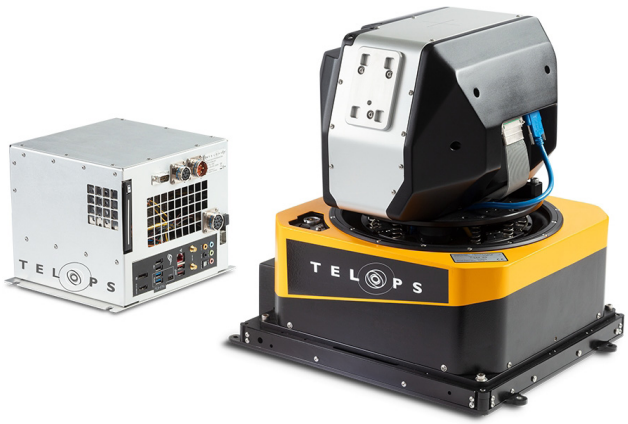
Intuitive SpArcfire operating software makes OES analysis quick and easy. The Hitachi GRADE Database, included in the OE720, offers more than 15 million records for over 340,000 materials from 74 countries and standards. Optional charge correction software automatically calculates the right quantity of material to add to a melt to bring it into spec. ExTOPE Connect wireless technology allows manufacturers to gather live data for real-time decision making even across multiple sites, lines and production stages.

Hitachi High-Tech

https://link.spectroscopyeurope.com/4147-P1-2021

IMAGING

Compact infrared hyperspectral camera



Telops has introduced a new compact hyperspectral imaging system, the Hyper-Cam Airborne Mini built on their existing Hyper-Cam. The Hyper-Cam Airborne Mini weighs 50 pounds (23 kg) and has a volume of roughly one cubic foot, enabling it to be installed into small aircraft. The Hyper-Cam Airborne Mini measures in the longwave infrared (7.4–11.8 µm) region. It can be used to spot indicator minerals during geological exploration missions, provide true signature measurement of military targets, detect gas leaks at an oil plant or quantify VOC emissions to support environmental compliance efforts.

In-flight operation of the Hyper-Cam Airborne Mini is controlled by the software that continuously adapts parameters to the flight conditions, and there is an active stabilisation platform coupled with an Image Motion Compensation system. Once in the air, the control and processing unit can automate the data

NEW PRODUCTS

acquisition process or allow the user to retain full control over acquisition parameters. An optional plug-in runs data analysis algorithms to present gas detection, identification and quantification results in real-time.

Telops

https://link.spectroscopyeurope.com/6346-P1-2021

INFRARED

FT-IR plastic analysis system

Shimadzu Scientific Instruments has introduced a new Fourier transform infrared (FT-IR) spectrophotometer plastic analysis system. The system uses Shimadzu's IRSpirit™ FT-IR spectrophotometer, QATR-S single-reflection ATR attachment and the Plastic Analyser Method Package. The Plastic Analyser method package includes FT-IR spectral libraries for plastics degraded by UV rays and heat. These libraries help investigators accurately analyse unknown samples that are difficult to identify with standard libraries. The UV-damaged plastics library includes more than 200 spectra from the UV degradation of 14 types of plastics, unirradiated and UV irradiated for 1–550 h. UV irradiation for 550 h with an ultra-accelerated weathering tester is equivalent to exposure to ultraviolet light for about 10 years. The thermal-damaged plastics library includes more than 100 spectra from the degradation of 13 types of plastic heated to between 200 °C and 400 °C.

Shimadzu Scientific Instruments

https://link.spectroscopyeurope.com/6348-P1-2021

MASS SPEC

Automatic sample injection system

Shimadzu has announced the release of the AOC-30 series of automatic sample injection systems for GC and GC/MS instruments. The new AOC-30 series helps ensure that anyone can operate the instrument and obtain expert-level results for routine analysis work in pharmaceutical, chemical and environmental fields. "Analytical Intelligence" functionality relieves operators from organisational, input and processing tasks. Functionality is included to support working from home or remotely, and includes features such as checking of system status and performing operations for everything from starting up the system to finishing analysis.

The AOC-30 series has several upgrade options. The AOC-30i Single Tower autoinjector carries 30 samples and provides intelligent wash possibilities with 4 different solvents. The AOC-30i Dual Tower features higher sample-throughput by simultaneous injection with two autoinjectors on one GC-2030. The combined AOC-30i autoinjector and AOC-20sU sampler cover an increased capacity of 150 vials.

Shimadzu

https://link.spectroscopyeurope.com/104-P1-2021

NEW PRODUCTS

Peptide LC-MS workflow

Waters has introduced a new peptide multi-attribute method (MAM) workflow for their BioAccord™ LC-MS system, enabling the monitoring of the efficacy and safety of monoclonal antibodies (mAbs) and other protein-based drugs. The peptide MAM workflow for the BioAccord System monitors for product variants, product degradation and impurities, and process stability-indicating modifications. The BioAccord System consists of the ACQUITY™ UPLC™ I-Class Plus with the ACQUITY RDa™ mass detector. In addition to peptide MAM, the BioAccord System also features workflows for other routine analyses of biotherapeutics: peptide mapping, intact/subunit mass analysis, released glycan profiling and oligonucleotide mass confirmation.

Waters

https://link.spectroscopyeurope.com/103-P1-2021

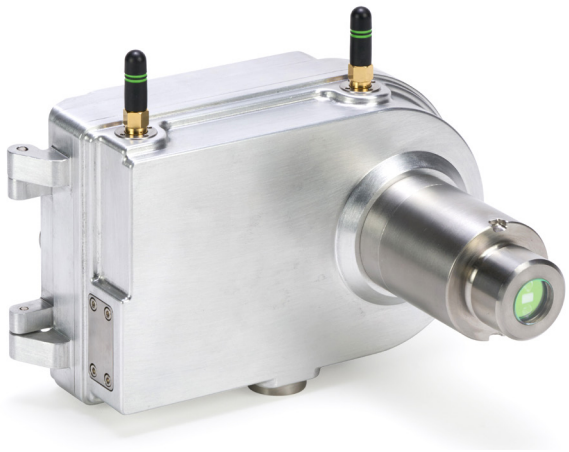
NIR

Viavi PAT-Wx NIR spectrometer

The PAT-Wx is the hazardous location version of Viavi's PAT-W wireless miniature process spectrometer. Its compact, lightweight design and automatic triggering function make it suitable for use on dynamic process equipment like tumble blenders. Since it is wireless and safe in the presence of flammable gases, vapours or dust, the PAT-Wx is also suited to diverse process monitoring applications in hazardous environments. As a member of the MicroNIR product family, it enables moving a process directly to production in a hazardous location using chemometric models and processes developed elsewhere. The PAT-Wx has a rechargeable Li-ion battery with >8 h of continuous run time, Wi-Fi connection to host via included router and integrated motion-sensitive triggering. It is washable (IP67- and IP65-rated enclosure), has an integrated PC for storing and forwarding collected spectral data and is compatible with all MicroNIR chemometric models.

Viavi

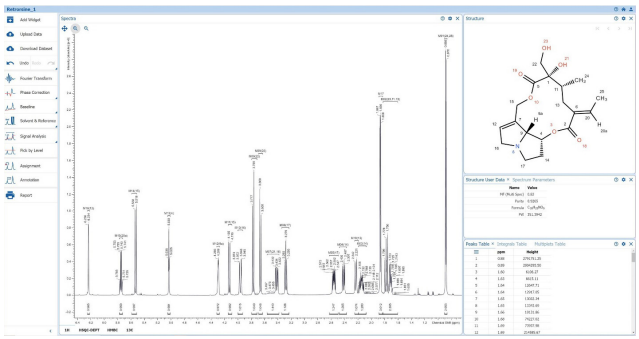
https://link.spectroscopyeurope.com/1764-P1-2021



NMR

Browser-based NMR processing application

ACD/Labs has launched a new browser-based application—Spectrus JS (for JavaScript). This new cross-platform application will work on Windows, macOS and Linux operating systems to process NMR data from all major NMR instrument vendors. Spectrus JS only requires access to a browser and internet connection to make NMR data processing and interpretation possible from anywhere. It introduces server-side processing for NMR and expands the cloud capabilities of the Spectrus platform with easy-to-deploy tools for remote working. The Spectrus



NEW PRODUCTS

platform supports all types of analytical techniques and has knowledge management and targeted workflow applications.
ACD/Labs

https://link.spectroscopyeurope.com/660-P1-2021

RAMAN

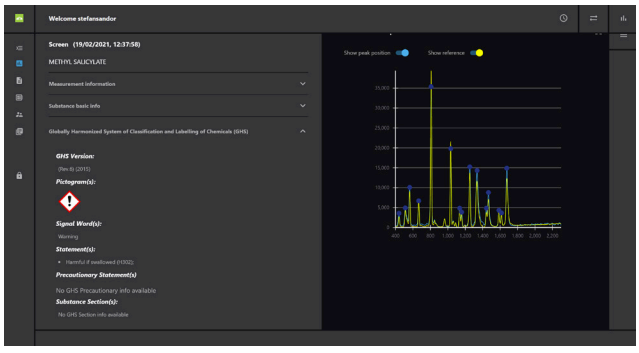
Raman bioprocess monitoring

A process analytical technology (PAT) solution has been introduced for real-time monitoring of bioprocesses without compromising the sterile boundary. SCHOTT, INFORS HT and tec5 have announced a product combination for the direct use of Raman spectroscopy in bioreactors. This is a combination of bioreactor, spectrometer system and probe receptacle, and meets typical instrumental and regulatory requirements. The new system integrates sensors into bioprocesses thanks to standardised interfaces. Measuring points can also be changed easily.

The system includes the bioreactor Minifors 2 and eve® bioprocess software from INFORS HT; the latter enabling users to centralise all bioprocess data in one database. Attached to the bioreactor port is the SCHOTT ViewPort™ sterile optical sensor receptacle. It features a hermetically sealed optical window made of sapphire for *in situ* process monitoring with optical sensors. Dedicated Raman spectrometer systems from tec5 have been specifically adapted to fit the different variants of SCHOTT's ViewPort™.

The ViewPort™ sensor receptacle can be attached to standard bioreactor ports, such as an ingold or PG13.5. The bioreactor and integrated ViewPort™ can then be sterilised as usual using γ-radiation or steam-in-place (SIP). Finally, the spectrometer probe is mounted with high positional accuracy on the ViewPort™ components during operation using a quick-release fastener. It is also easy and safe to change the probe between different ports. All components are manufactured using materials in accordance with pharma industry best practices, making the system ideally suited for use in regulated areas, such as Good Manufacturing Practice (GMP) and hygienic design.
SCHOTT

https://link.spectroscopyeurope.com/6345-P1-2021



Serstech launches a new Raman software platform

Serstech has launched a new software platform which replaces the previous ChemDash One PC application. The new platform is initially made up of three applications: ChemDash Lite, ChemDash Pro and ChemDash Pro+. The Lite version is included for free with Serstech's instruments as a direct replacement for ChemDash One. ChemDash Pro is a premium application that is sold either separately or together with any of Serstech's instruments. The application includes enterprise functionality that makes the application easier to deploy throughout customer

organisations. ChemDash Pro+ is compliant with US FDA's regulatory framework for pharmaceutical production.
Serstech
https://link.spectroscopyeurope.com/6336-P1-2021

RELATED EQUIPMENT

Passive sampler for VOC analysis

Markes International has launched a next-generation passive sampler that combines all the benefits of radial and axial VOC samplers, and which the company says will ultimately make large scale air monitoring studies easier to run and more affordable. The Pocket Diffuser Sampler (POD Sampler) provides better sensitivity, higher accuracy and faster response times, whilst also improving on ease of use and re-usability compared to other passive samplers. The POD cartridges can be reconditioned and reused over 100 times and the sampler itself can be used indefinitely. The POD Sampler was developed in partnership with the European Commission's Joint Research Centre (JRC) in Ispra, Italy, the European reference laboratory for air pollution. The POD Sampler is compatible with any commercial thermal desorption system.
Markes International
https://link.spectroscopyeurope.com/681-P1-2021

UV/VIS

UV-visible-NIR spectrophotometer for a microscope

CRAIC Technologies has introduced the 508 PV™ UV-visible-NIR spectrophotometer that is designed to be added to an open photoport of a microscope or probe station to non-destructively analyse the spectra of many types of microscopic samples. The 508 PV™ can acquire spectra of microscopic sample areas by absorbance, reflectance, polarisation, luminescence and fluorescence, in addition to high-resolution colour images, when attached to properly configured microscopes. The 508 PV™ spectrophotometer integrates CRAIC Technologies Lightblades™ spectrophotometer with optical interface hardware and easy-to-use Lambdafire™ software. Lightblades™ are spectrophotometers specifically designed for microscale analysis.
CRAIC Technologies
https://link.spectroscopyeurope.com/3247-P2-2021

NEW PRODUCTS

X-RAY

Cloud-based monitoring of XRF spectrometers

Malvern Panalytical has introduced Smart Manager, a cloud-based dashboard that connects and monitors all Zetium and Axios-^{mAX} XRF systems. It will give customers a picture of both the real-time utilisation and health of their instruments, wherever they are in the world. Smart Manager also continually analyses data, monitoring many instrument variables and flagging anomalies in real time.

Malvern Panalytical

https://link.spectroscopyeurope.com/690-P1-2021

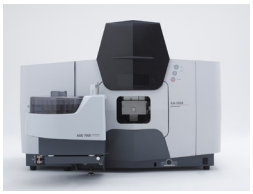
Product Focus on Atomic Spectroscopy

Shimadzu Europa GmbH	Tel: +49-203-76870 shimadzu@shimadzu.eu www.shimadzu.eu	SHIMADZU Excellence in Science

PRODUCT: AA-7000 Series

APPLICATIONS: Trace metal analysis e.g. in cosmetics; food water; drugs; blood; oil or petroleum

KEY FEATURES: High-sensitivity & fast analysis of trace metals; modular system flame and/or graphite furnace; compact footprint for user-friendly operation; 3D double-beam optics; full range of safety mechanisms



Conferences

2021

25–28 April, Oviedo, Spain. **5th International Glow Discharge Spectroscopy Symposium (IGDSS2021).** pete@masscare.co.uk, https://www.ew-gds.com/forthcoming-events/

23–26 May, Baeza (Jaen), Spain. **2nd Workshop-Symposium VitroGeowastes: Vitrification, Geopolymerization, Wastes Management and Circular Economy.** lperezvi@ujaen.es, http://vitrogeowastes.com

20–24 June, Duesseldorf, Germany. **51st International Symposium on High Performance Liquid Phase Separation and Related Techniques.** Michael Lammerhofer, michael-laemmerhofer@uni-tuebingen.de, https://www.hplc2021-duesseldorf.com/

18–23 July, Boston, MA, United States. **XXIX International Conference on Magnetic Resonance in Biological Systems (ICMRBSXXIX).** https://www.icmrbs2020.org

1–6 August, Freiberg (Sachsen), Germany. **Geoanalysis 2021.** geoanalysis2021@hzdr.de, https://geoanalysis2021.de

22–27 August, Krakow, Poland. **11th International Conference on Advanced Vibrational Spectroscopy (ICAVS 11).** icavs2021@targi.krakow.pl, http://www.icavs.org/gb/

6–10 September, Heraklion, Crete, Greece. **NanoBio Conference 2021.** info@nanobioconf.com, https://nano-bioconf.com

20–24 September, Online. **11th International Workshop on Infrared Microscopy and Spectroscopy with Accelerator Based Sources.** WIRMS2021@spring8.or.jp, http://www.spring8.or.jp/en/WIRMS2021/

18–20 October, Trondheim, Norway. **2nd Nordic Metabolomics Conference.** mila.knoff@ntnu.no, https://www.ntnu.edu/isb/nmc2021

31 October–4 November, Philadelphia, PA, United States. **69th ASMS Conference.** https://www.asms.org/conferences/annual-conference/future-annual-conferences

16–20 December, Honolulu, Hawaii, United States. **The International Chemical Congress of Pacific Basin Societies 2021.** https://pacifichem.org

2022

31 May–2 June, Kristiansand, Norway. **10th World Conference on Sampling and Blending (WCSB10).** contact@wcsb10.com, https://wcsb10.com

5–9 June, Minneapolis, Minnesota, United States. **70th ASMS Conference.** https://www.asms.org/conferences/annual-conference/future-annual-conferences

4–7 July, Skagen, Denmark. **International Association for Spectral Imaging (IASIM).** 2020@iasim.net, https://2020.iasim.net

2023

29 January–3 February, Ljubljana, Slovenia. **2023 European Winter Conference on Plasma Spectrochemistry.** Johannes T. VanElteren, http://www.ewcps2021.ki.si

Courses

2021

7–9 June, Online. **X-ray Photoelectron Spectroscopy (XPS) and Data Processing Short Course.** j.grant@ieee.org, https://surfaceanalysis.org/Online_Short_Courses.html

10–11 June, Online. **Computer Aided Surface Analysis for X-ray Photoelectron Spectroscopy (CAsaXPS) Short Course.** j.grant@ieee.org, https://surfaceanalysis.org/Online_Short_Courses.html

Exhibitions

2021

23–25 September, Hyderabad, India. **analytica Anacon India and India Lab Expo.** sheron.david@mm-india.in, https://www.analyticaindia.com/

15–17 November, Dubai, United Arab Emirates. **ARABLAB 2021.** info@arablab.com, https://www.arablab.com

2021

5–9 March, Atlanta, GA, USA. **Pittcon 2022.** https://www.pittcon.org

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Introduction to the Theory and Practice of Sampling

Kim H. Esbensen

with contributions from Claas Wagner, Pentti Minkkinen, Claudia Paoletti, Karin Engström, Martin Lischka and Jørgen Riis Pedersen

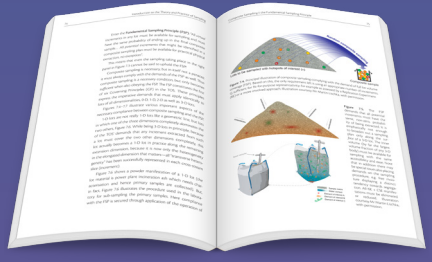
"Sampling is not gambling". Analytical results forming the basis for decision making in science, technology, industry and society must be relevant, valid and reliable. However, analytical results cannot be detached from the specific conditions under which they originated. Sampling comes to the fore as a critical success factor before analysis, which should only be made on documented representative samples. There is a complex and challenging pathway from heterogeneous materials in "lots" such as satchels, bags, drums, vessels, truck loads, railroad cars, shiploads, stockpiles (in the kg–ton range) to the miniscule laboratory aliquot (in the g–µg range), which is what is actually analysed.

This book presents the Theory and Practice of Sampling (TOS) starting from level zero in a novel didactic framework without excessive mathematics and statistics. The book covers sampling from stationary lots, from moving, dynamic lots (process sampling) and has a vital focus on sampling in the analytical laboratory.

"I recommend this book to all newcomers to TOS"

"This book may well end up being the standard introduction sourcebook for representative sampling."

"One of the book's major advantages is the lavish use of carefully designed didactic diagrams"



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