Vol. 33 No. 1 February 2021

SPECTROSCOPY europe

Spectroscopy since 1975

fNIRS shows chocolate is good for the brain

Atomic spectrometry traceable measurements

Virtual events: experience and their future

IMPOpen

Some good news at last! It appears that chocolate is good for the brain. Discover your excuses in the News article on page 4.

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EDITORIAL

It seems ages since I wrote my last Editorial, announcing the change to purely digital publication. So much has happened in the World with ups and downs of the COVID-19 pandemic and political changes. Now, we are here with Issue 1 of the new digital era. We have learnt a lot, and have much more to learn, about the opportunities purely digital publication brings for interactivity. It is easy to add unnecessary enhancements just for the sake of doing so, and we will try and avoid that. However, we also need to try things to see if they have real value. So, please bear with us.

What has not changed with purely digital production is our aim to bring you content/information that will interest and inform you. It has always been a challenge when spectroscopy has such a broad range of applications and individual techniques. Considering the type of content we are publishing, our current offering seems to be popular in the Reader Survey. Articles and columns, news, and new products were all clearly appreciated. Our Top 20 in 2020 offering showed the wide range of content that caught your eyes: from COVID-related columns, news and applications to environmental concerns, to the latest instrumentation. I hope what we publish in 2021 will be of even greater interest.

I was slightly surprised with the high proportion of people who wanted to read digital issues on a desktop or laptop computer. However, perhaps this is linked to the preference for PDF (see below). Mobile phones and paper were a long way back, with tablets even further back.

As to format, PDF was a clear winner, followed by pages on a website and a flipbook. An app for a mobile device only attracted 10 %, although 17 % want to read issues on a smartphone! When asked what they would like to read if they had to choose just one format, PDF pulled even further ahead.

It would have been quite easy to just provide a PDF ready to print, but I was keen to keep as many readers happy as possible. So, initially there will be three formats:

- PDF: ready to print out or to read on screen
- Flipbook, with some additional interactivity; good for tablets
- Mobile: an HTML5 version that you open with the browser on your smartphone.

These three editions should cover >90 % of readers' requests. We are learning a lot about digital formats and welcome your feedback! The survey is still open and I would encourage you to complete it if you have not already done so (spectroscopyeurope.com/2021-survey).

Ian Michael

fNIRS shows chocolate is good for the brain

The brains of healthy adults recovered faster from a mild vascular challenge and performed better on complex tests if the participants consumed cocoa flavanols beforehand, researchers report in *Scientific Reports* (doi.org/ghmtwv). In the study, 14 of 18 participants saw these improvements after ingesting the flavanols. Previous studies have shown that eating foods rich in flavanols can benefit vascular function, but this is the first to find a positive effect on brain vascular function and cognitive performance in young healthy adults, said Catarina Rendeiro, from the University of Birmingham who led the research with University of Illinois at Urbana-Champaign psychology professors Monica Fabiani and Gabriele Gratton.

"Flavanols are small molecules found in many fruits and vegetables, and cocoa, too", Rendeiro said. "They give fruits and vegetables their bright colours, and they are known to benefit vascular function. We wanted to know whether flavanols also benefit the brain vasculature, and whether that could have a positive impact on cognitive function."

The team recruited adult non-smokers with no known brain, heart, vascular or respiratory disease, reasoning that any effects seen in this population would provide robust evidence that dietary flavanols can improve brain function in healthy people. The team tested the 18 participants before their intake of cocoa flavanols and in two separate trials, one in which the subjects received flavanol-rich cocoa and another during which they consumed processed cocoa with very low levels of flavanols. Neither the participants nor researchers knew which type of cocoa was consumed in each of the trials. This double-blind study design prevents researchers' or participants' expectations from affecting the results.

About two hours after consuming the cocoa, participants breathed air with 5 % CO_2—about 100 times the normal concentration in air. This is a standard method for challenging brain vasculature to determine how well it responds, Gratton said. The body typically reacts by increasing blood flow to the brain, he said: "this brings in more oxygen and also allows the brain to eliminate more carbon dioxide".

Using functional near infrared spectroscopy (fNIRS), the team measured oxygenation in the frontal cortex, a brain region that plays a key role in planning, regulating behaviour and decision-making.

"This allows you to measure how well the brain defends itself from the excess carbon dioxide", Fabiani said.

Researchers also challenged participants with complex tasks that required them to manage sometimes contradictory or competing demands. Most of the participants had a stronger and faster brain oxygenation response after exposure to cocoa flavanols than they did at baseline or after consuming cocoa lacking flavanols, the researchers found.

"The levels of maximal oxygenation were more than three times higher in the high-flavanol cocoa versus the low-flavanol cocoa, and the oxygenation response was about one minute faster", Rendeiro said.

After ingesting the cocoa flavanols, participants also performed better on the most challenging cognitive tests, correctly solving problems 11 % faster than they did at baseline or when they consumed cocoa with reduced flavanols. There was no measurable difference in performance on the easier tasks, however.

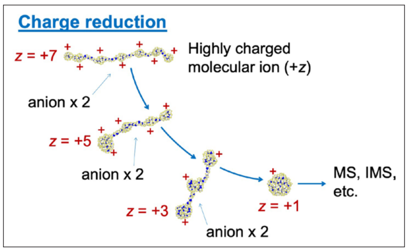
"This suggests that flavanols might only be beneficial during cognitive tasks that are more challenging", Rendeiro said.

Participants varied in their responses to cocoa flavanols, the researchers found. "Although most people benefited from flavanol intake, there was a small group that did not", Rendeiro said. Four of the 18 study subjects had no meaningful differences in brain oxygenation response after consuming flavanols, nor did their performance on the tests improve. "Because these four participants already had the highest oxygenation responses at baseline, this may indicate that those who are already quite fit have little room for improvement", Rendeiro said. "Overall, the findings suggest that the improvements in vascular activity after exposure to flavanols are connected to the improvement in cognitive function."

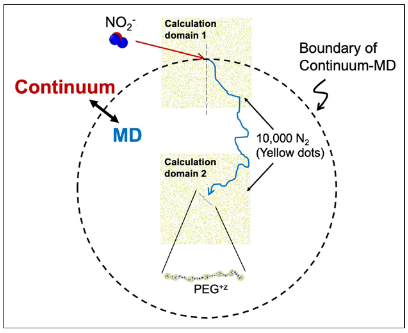
Computer simulations improve mass spectrometry

A team of researchers lead by Kanazawa University have used a powerful molecular dynamics simulation to better understand the effect of excess charges on molecules tested by a mass spectrometer. They modelled the effect of adding molecules of the opposite charge in order to neutralise excess charge. In this case, the positive charge on polyethylene glycol (PEG) can be reduced via collision with negatively charged NO_2^- ions.

However, this is complicated by the fact that the likelihood of colliding depends on the amount of charge in the first place. "Charged polymers can adopt charge-state dependent structures because of electrostatic stretching", first author Tomoya Tamadate says. For example, with small excess charge, PEG assumes a compact form. However, as the charge increases, the mutual repulsion between the positive charges causes it to straighten out.



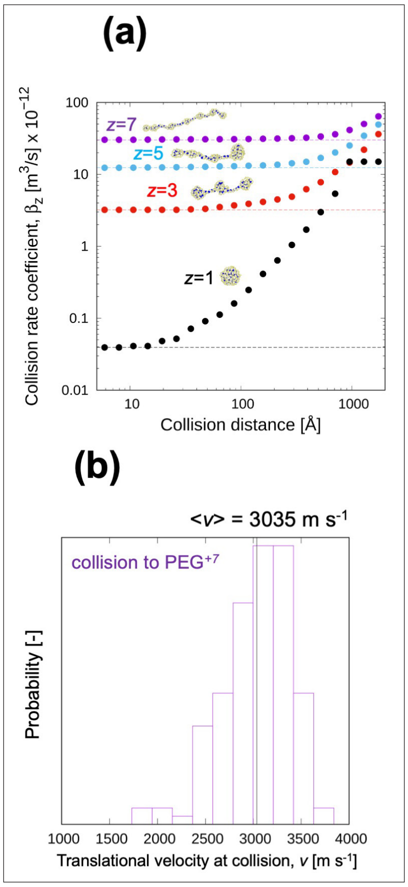
A depiction of a charge reduction process which is utilised as a pre-treatment process for mass spectrometry or ion mobility spectrometry. To increase the accuracy of the spectrum, excess charges on the molecular ion (PEG in this figure) are removed via collision with anion in gas.



An outline of the developed calculation model (continuum-molecular dynamics simulation hybrid method). In this model, when the inter-ion distance is sufficiently large, relative motion is described by diffusion equations (continuum), meanwhile within a specific distance (shown as a broken line), molecular dynamics (MD) simulations are utilised to calculate the trajectory. In order to decrease the calculation cost, they perform the MD simulation with gas molecules only arranged around the target ions.

To help speed up the calculations, the team used the "continuum approximation" method, which only starts simulating all of the atoms in the NO_2^- molecule once it approaches close enough to the PEG.

"The success of this project shows that hybrid continuum-molecular dynamics simulations can be used more generally to study collision-driven reactions molecules that can take on different conformations", senior author Takafumi Seto says. The results can lead to more effective methods of controlling excess charge in sample molecules, which will allow for more accurate results.



(a) The recombination (collision) rate coefficient of the PEG ion with different numbers of charges. This collision rate coefficient showed good agreement with the experimentally measured charge reduction rate. (b) Translational velocity distribution of NO_2^- ion at collision. We expect the kinetic energy can be used to evaluate the possibility of collision-induced reaction.

The work has been published in *Physical Chemistry Chemical Physics* (doi.org/fsg9).

Quantum-limit-approaching chemical sensing SERS chip

University at Buffalo researchers have reported an advancement of a chemical sensing chip based on surface-enhanced Raman spectroscopy (SERS) that could lead to handheld devices that detect trace chemicals. The chip, which may have uses in food safety monitoring, anti-counterfeiting and other fields where trace chemicals are analysed, is described in a study that was published in *Advanced Optical Materials* (doi.org/fshb).

"There is a great need for portable and cost-effective chemical sensors in many areas, especially drug abuse", says the study's lead author Qiaoqiang Gan, professor of electrical engineering in the UB School of Engineering and Applied Sciences. The work builds upon previous research Gan's lab led that involved creating a chip that traps light at the edges of gold and silver nanoparticles. While effective, the earlier chip wasn't uniform in its design. Because the gold and silver were spaced unevenly, it could make scattered molecules difficult to identify, especially if they appeared on different locations of the chip.

Gan and a team of researchers—featuring members of his lab at UB and researchers from the University of Shanghai for Science and Technology in China, and King Abdullah University of Science and Technology in Saudi Arabia—have been working to remedy this shortcoming. The team used four molecules (BZT, 4-MBA, BPT and TPT), each with different lengths, in the fabrication process to control the size of the gaps in between the gold and silver nanoparticles. The

Company News

Camo acquired by Aspen Technology

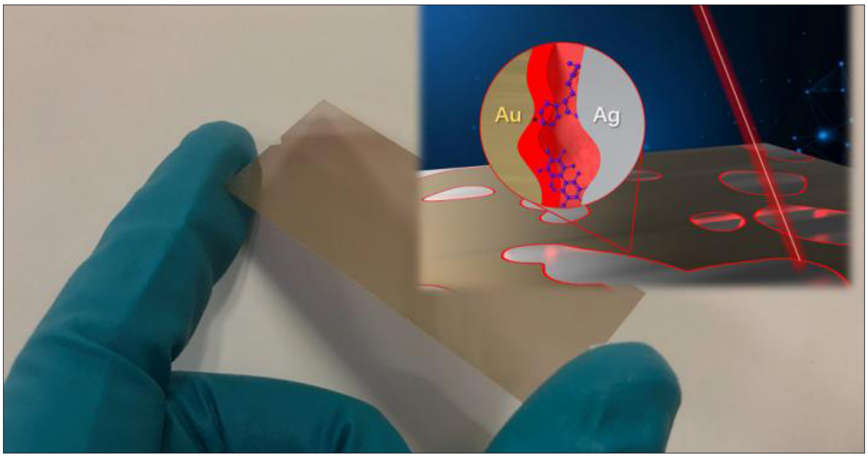
Camo Analytics, producer of the Unscrambler chemometrics software, has been acquired by Aspen Technology, Inc. Camo's products will strengthen AspenTech's portfolio with Process Analytical Technology (PAT) and Overall Equipment Effectiveness (OEE) solutions to meet compliance requirements.

Antonio Pietri, president and chief executive officer of Aspen Technology commented, "Camo Analytics is a great addition to our portfolio and supports the expansion of our capabilities to the pharmaceuticals industry and several other industries. We were impressed by the depth of knowledge and drive for innovation from the Camo Analytics team and look forward to continuing investment in the solutions and bringing them to new customers and markets."

Raman Bhatnagar, chief executive officer for Camo Analytics commented: "On behalf of the Camo Analytics team, I am very happy to see us become part of a global leader in digital transformation. We share the same vision that the ability to analyse data from across the organisation and effectively predict behaviours are critical to achieving the smart enterprise of the future. Bringing our technology to the Industrial AI of AspenTech is very exciting."

The entire Camo team is now part of AspenTech and they confirm it is business as usual, now with more resources and a broader set of solutions to accelerate product development. Camo's office remains in Oslo.

Chairman of the board Erik Langaker and CEO Raman Bhatnagar of Camo Analytics.



The SERS chip, which also may have uses in food safety monitoring, anti-counterfeiting and other fields where trace chemicals are analysed. Credit: Huaxiu Chen, University at Buffalo.

updated fabrication process is based upon two techniques, atomic layer deposition and self-assembled monolayers, as opposed to the more common and expensive method for SERS chips, electron-beam lithography.

The result is a SERS chip with unprecedented uniformity that is relatively inexpensive to produce. More importantly, it approaches quantum-limit sensing capabilities, says Gan, which was a challenge for conventional SERS chips

"We think the chip will have many uses in addition to handheld drug detection devices", says the first author of this work, Nan Zhang, PhD, a postdoctoral researcher in Gan's lab. "For example, it could be used to assess air and water pollution or the safety of food. It could be useful in the security and defence sectors, and it has tremendous potential in health care."

Mass spectrometry to test for bovine mastitis

A research project to tackle bovine mastitis and reduce the use of broad-spectrum antibiotics on dairy farms—and so potentially help in the fight against antimicrobial resistance (AMR)—is underway at the Institute for Global Food Security (IGFS), Queen's University Belfast, UK, in partnership with AgriSearch and AFBI. The new approach will involve the use of mass spectrometry to develop a rapid diagnosis of mastitis, directly from a suspected milk sample. This will initially use laboratory-based equipment but could potentially be translated to an on-site test to further increase test turnaround times. The project will also explore the potential for the wider application of rapid evaporative ionisation mass spectrometry (REIMS) in areas such as milk-quality analysis and the monitoring of lameness in herds.

Bovine mastitis is a painful inflammatory condition of the udder, caused by the cow's immune response to a microbial infection. It is a significant challenge to the dairy farmer and to the industry due to the effect on cow health and welfare, the complexities of controlling the condition and the need to withhold milk from human consumption during treatment and recovery.

Farmers carry out a visual inspection of the milk as part of the milking process; changes, such as the formation of clots in the milk, can be indicative of clinical mastitis in addition to the direct observation of heat or swelling of the udder. "Somatic cell counting" of a milk sample can be useful in screening for pre-clinical mastitis, particularly where farmers regularly undertake milk recording of their herd. Microbial culture and sensitivity are then carried out to determine the causal pathogen and the best type of antibiotic treatment, but these tests can take several days and rely on an uncontaminated sample being collected in the milking parlour.

Broad-spectrum antibiotic treatment is usually started immediately, before microbiology results have been returned by the laboratory, to minimise the pain and suffering of the cow, but such therapeutic use of broad-spectrum antibiotics has the potential to contribute to AMR—an increasing problem for both animal and human health.

The REIMS approach, however, could eliminate the need for time-consuming milk-sample preparation and, therefore, be more user-friendly for farmers with near-instantaneous results. Additionally, the rapid identification of pathogens would allow for more timely, targeted "narrow-spectrum" treatments, potentially reducing the use of broad-spectrum antibiotics. In fact, if rapid diagnostics also facilitated earlier treatment, the use of antibiotics might be eliminated altogether, further helping society's battle against AMR.

As part of a PhD project at IGFS and the School of Biological Sciences, milk samples will be collected from dairy farms which are part of the AgriSearch network and, through AFBI, from cows with suspected and confirmed mastitis, alongside healthy control samples. The same project will also look at lameness in dairy cattle. Current diagnosis of lameness involves visual observation which unfortunately means cows are often undiagnosed until the problem has become fairly advanced. A longitudinal study to assess a naturally occurring molecule or gene will be conducted on a dairy herd using REIMS so as to identify potential biomarkers that could flag up a proclivity towards lameness.


Photo by Og Mpango on Unsplash

Mass spec reveals more of the dangers of forest fires

Researchers from Yale University have taken samples of smoke from forest fires from an aeroplane and analysed them offline with high-resolution tandem mass spectrometry. This has produced a highly detailed look at the chemical make-up and transformations of an evolving plume of forest fire smoke—findings that could contribute to a better understanding of air pollution in many parts of the world.

The results show clear evidence for the formation of particle-phase organic compounds containing oxygen, nitrogen and sulfur. They also found that certain structural features that were part of these compounds increased significantly as the smoke plume evolved over a period of four hours. The study is published in *Atmospheric Chemistry and Physics* (doi.org/fshd).

Previous studies have used mass spectrometry to study wildfire smoke. However, they have not fully captured these complex compounds and their chemical transformations in these smoke plumes. The Yale researchers used a unique approach of high-resolution tandem mass spectrometry for a more precise analysis of the evolving smoke

Konica Minolta to acquire Specim

Konica Minolta Sensing Europe BV has entered into a definitive agreement to acquire Specim, Spectral Imaging Oy Ltd. Specim has been supported by two Finnish investors, Nordic Option (since 2015) and Bocap (since 2017). Both investors welcome Konica Minolta as an acquirer, as this step forms part of a continuum of evolution for Specim. In the spring of 2020, Specim's investors and founders initiated a competitive trade sale process resulting in offers from several global players. Of these, the Board determined Konica Minolta to be the perfect home for Specim's technology, customers and employees. The acquisition is expected to fuel Specim's growth in global industrial markets. Upon acquisition, Specim will maintain its existing offices and facilities in Oulu.

New MD at Specac

Shannon Postma has been appointed as Managing Director of Specac Limited. Shannon joins the business as the previous MD, David Smith, assumes the new role of Commercial Director. David will remain on the Board of Directors and will focus his effort on driving commercial success in new application areas including in the diagnostics, analytics and life sciences markets.

Shannon is an Australian national who has led, grown and sold businesses with attributes similar to Specac. He was most recently General Manager of The Galloway Group, a diversified group of Australian SMEs and is an experienced commercial and operational leader; both being focus areas for Specac over the next five years as it becomes a larger, more sophisticated business.

Shannon Postma, new MD at Specac

plume. This level of detail is an important step toward improving modelling capabilities and our understanding of the health and environmental impacts of biomass burning smoke.

Knowing the precise make-up of the smoke of these fires is particularly important, since it is predicted that forest fires will become increasingly prevalent and severe due to climate change. The results from this wildfire-focused study chemical pathways are also relevant to places in developing regions or very large cities where residential biomass burning is common.

"It provides evidence for the formation of these understudied organic compounds with oxygen, nitrogen and sulfur that are likely to be relevant in other regions with substantial biomass and fossil fuel combustion, such as large cities in the developing world", Drew Gentner, associate professor of chemical & environmental engineering, said. "Along with other researchers, we've seen significant amounts of these compounds at other field sites in the past, but often wonder about their formation pathways and underlying chemical structures, and this real-world biomass burning plume provided a great opportunity to study them."

The study is part of an ongoing collaboration between Gentner's lab with Environment & Climate Change Canada, the national environmental agency.

Samples were collected during two aircraft research flights by Environment & Climate Change Canada as part of its air pollution research programme. These flights sampled two boreal forest wildfire smoke plumes that originated near Lac La Loche in northern Saskatchewan. The fire was a low-intensity surface fire with smouldering conditions. The particles were collected onto filters, placed in a deep freezer and sent to Gentner's lab.

Another tilt at the non-invasive glucose monitoring windmill?

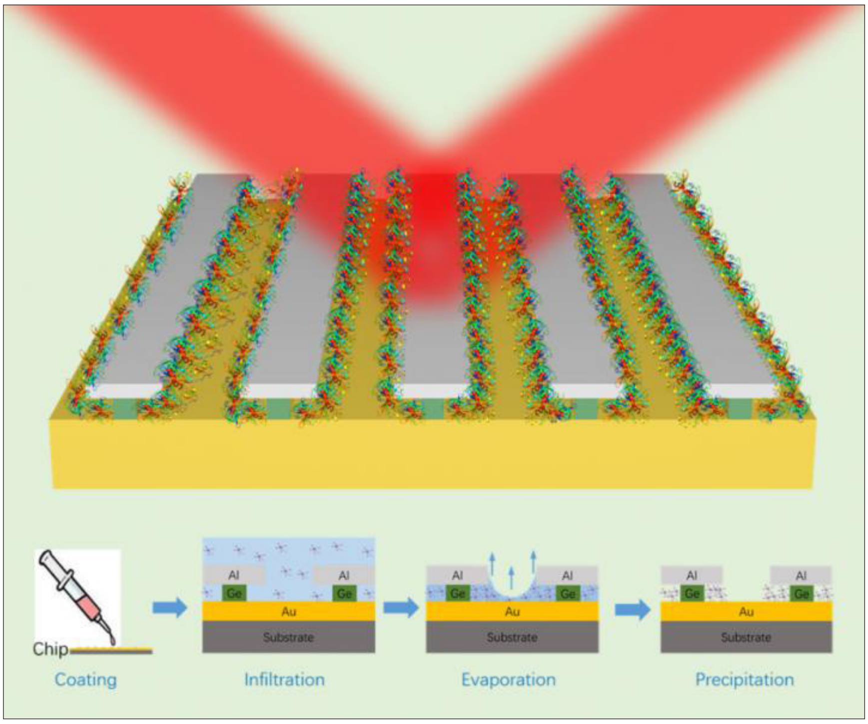
Quantum Operation Inc. (https://quantum-op.co.jp/en) is a Japanese healthcare IoT startup, who presented their non-invasive glucose monitor that is capable of continuous measurement at the giant Consumer Electronics Show (CES). The device can be worn on the wrist and can provide continuous monitoring. Other sensors such as oxygen saturation and electrocardiography are also being developed.

Details are (very) scarce but they do say they are using "spectrometer materials".

High-sensitivity SEIRA sensors using passive trapping of analyte molecules

In a paper published in *Light: Science & Applications* (doi.org/fsw6), a team of scientists, led by Dr Peter Q. Liu from the State University of New York at Buffalo, have demonstrated a new type of high-performance optical sensor which can utilise the surface tension of liquid to concentrate and trap analyte molecules at the most sensitive locations of the device structure, and hence significantly enhance the sensitivity performance. Based on a metal-insulator-metal sandwich structure which also features nanometre scale trenches, the sensor can passively retain and concentrate an analyte solution in these trenches as the solution gradually evaporates on the sensor surface, and eventually trap the precipitated analyte molecules inside these trenches. As the light intensity is also highly enhanced in these trenches by design, the interaction between light and the trapped analyte molecules is drastically enhanced, leading to a readily detectable optical signal (i.e. changes in the light absorption spectrum) even at the picogram level.

In general, the absorption of infrared light is intrinsically weak, optical sensors can drastically enhance the molecular absorption by employing suitable nanostructures on the device surface to confine light into very small volumes (so called hot-spots), which leads to very large light intensity. In doing so, each molecule in the hot-spots can absorb much more light in a given time interval than a molecule outside the hot-spots, which makes it possible to measure very low quantity of chemical or biological substances with high reliability, if enough



Top: schematic of the optical sensor design with trapped molecules. Bottom: schematic showing the process of concentrating and trapping molecules in a solution. Credit: Xianglong Miao, Lingyue Yan, Yun Wu and Peter Q. Liu

molecules are located in the hot-spots. This general approach is also called surface enhanced infrared absorption (SEIRA).

However, a key issue for most SEIRA optical sensors is that the hot-spots only occupy a tiny portion of the entire device surface area. On the other hand, the analyte molecules are usually randomly distributed on the device surface, and hence only a small fraction of all analyte molecules are located in the hot-spots and contribute to the enhanced light absorption. "The SEIRA signal would be much larger if most of the analyte molecules can be delivered into the hot-spots of an optical sensor. This is the key motivation of our optical sensor design", Dr Liu said.

"There are techniques, such as optical tweezers and dielectrophoresis, which can manipulate small particles or even molecules and deliver them to target locations such as the hot-spots. However, these techniques require significant amount of energy input and are also complicated to utilise." Dr Liu added, "what we set out to explore is a device structure that can trap analyte molecules precipitated out of a solution into the hot-spots in a passive (requiring no energy input) and effective way, and we realised that we can make use of the surface tension of liquid to achieve this goal."

In addition to the demonstration of high-sensitivity biomolecule sensing, the team also conducted another set of experiments, which showed that the same type of device structure also achieved effective trapping of liposome particles (typically ~100 nm) in the tiny trenches. This means such optical sensors can be optimised for detecting and analysing nano-objects such as viruses or exosomes, which have similar sizes to the liposomes used in the experiments.

The team believes that the demonstrated SEIRA optical sensor design strategy can be applied to other types of optical sensors as well. Besides sensing applications, such device structures can also be used for manipulating nanoscale objects including exosomes, viruses and quantum dots.

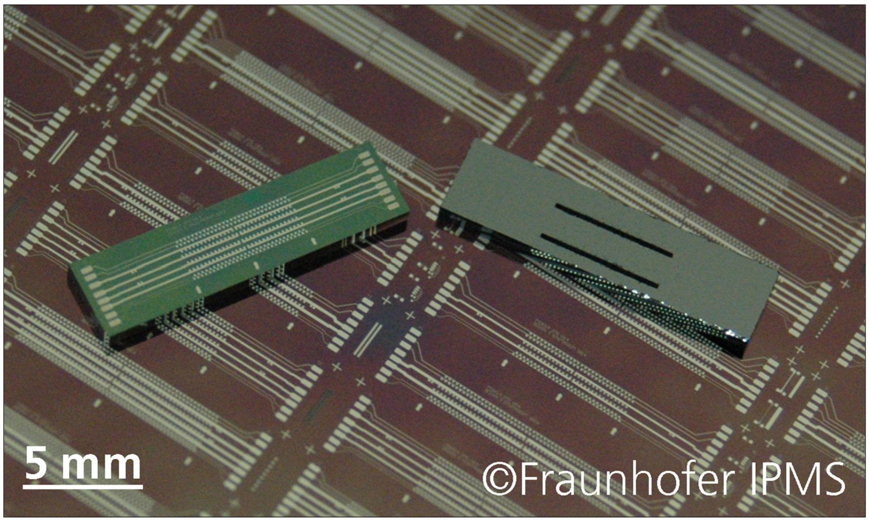
David Birch honoured for pioneering UK fluorescence lifetime industry

HORIBA Scientific has announced that David Birch has been awarded the 2020 Dennis Gabor Award by the Institute of Physics (IOP). Dr Birch is an Emeritus Professor of Photophysics at the University of Strathclyde and a founding Director of HORIBA Jobin Yvon IBH Ltd, one of the earliest corporate spin-offs in Scotland. His contributions in the fluorescence sector included research on techniques, multi-disciplinary applications and developing instrumentation for measuring fluorescence lifetimes, including the TCSPC (Time-correlated Single-Photon Counting) technique.

The Dennis Gabor Medal, named for the inventor of holography and 1971 Nobel Prize winner, is awarded for distinguished contributions to the application of physics in industry.

As Chairman at IBH, Dr Birch pioneered TCSPC fluorescence lifetime spectroscopy and his recent research has focused on the application of fluorescence to molecular grand challenges at the biomedical interface. He championed the merger of IBH and HORIBA. He has published over 250 peer-reviewed journal articles, and his contributions to research and new products have been recognised through Fellowships of the IOP, the Royal Society of Edinburgh, the Royal Society of Chemistry and Visiting Chairs at Texas Christian University, Kyoto Institute of Technology, the Czech Technical University and the University of Madras. Presently he is co-founding Editor-in-Chief of IOP's *Methods and Applications in Fluorescence*.

David Birch



At the heart of the ion-mobility spectrometer is a miniaturised FAIMS chip. © Fraunhofer IPMS

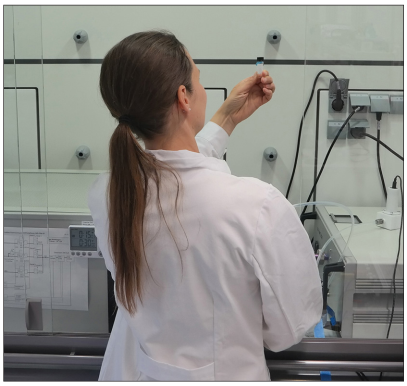
Ion mobility spectrometry to detect cancer from exhaled breath

Researchers at the Fraunhofer Project Hub for Microelectronic and Optical Systems for Biomedicine MEOS are now developing solutions designed to enable the analysis of breath gas for the diagnosis of disease. Although their research focuses on the early detection of cancer, the same principle could also be applied to distinguish between COVID-19 and other respiratory diseases.

"A lot of diseases cause a change in the composition of the volatile organic trace gases in exhaled air that can be used as biomarkers", explains Dr Jessy Schönfelder, research associate at Fraunhofer MEOS. "It's often a combination of several trace gases in a significantly elevated or significantly reduced concentration that is characteristic for a specific disease. This is known as the VOC fingerprint or VOC pattern." Fraunhofer MEOS in Erfurt is an interdisciplinary project hub involving the participation of the Fraunhofer Institutes for Cell Therapy and Immunology IZI, Photonic Microsystems IPMS, and Applied Optics and Precision Engineering IOF.

The team are developing an ion-mobility spectrometry (IMS) instrument with which to identify these VOC patterns. At the heart of the IMS system is a miniaturised high-field asymmetric ion mobility spectrometry (FAIMS) chip. The microelectromechanical system comprises an ion filter and a detector. The device also features a UV lamp. In the first instance, the VOCs, borne in a carrier gas, are pumped into the spectrometer, where they are ionised by UV light. "These are then fed to the FAIMS chip, which was developed by Fraunhofer IPMS", says Schönfelder. "An alternating voltage is then applied at the filter electrodes. By adjusting the voltage at the filter, you can control which VOCs get through to the detector. This generates a VOC fingerprint, which enables us to identify the disease we're looking for."

The research team at Fraunhofer MEOS hopes this new technology will be able to detect a broad range of biomarkers. They also want to use it to distinguish between COVID-19 and other respiratory infections. It likewise features in the Fraunhofer cluster project M3Infekt, which is developing a mobile, modular, multimodal monitoring system to enable rapid intervention in the event of a sudden deterioration in the condition of COVID-19 patients. Furthermore, it is hoped that this method of breath gas analysis might provide an advance indication of neurodegenerative diseases such as Alzheimer's. This would not only provide earlier warning than with conventional methods such as blood testing but also be more convenient, since it merely requires that the patient breathe into a tube.



Dr Jessy Schönfelder with gas-measurement equipment (left) and a reference instrument for gas analysis (right). © Fraunhofer MEOS

"There's huge potential for sensor systems in breath gas analysis", Schönfelder explains. "IMS technology is non-invasive, sensitive and selective. And it is quick, inexpensive and also compact and portable, so there's no reason why it shouldn't be used in medical practices and hospitals. The finished product will be about the size of a shoebox."

At present, the research team is working to enhance the instrument's electronic control system and to improve sample extraction and sample processing. Meanwhile, reference measurements with cell cultures have now been successfully conducted, and further investigations with clinical human samples are in the pipeline. In a project recently completed at Fraunhofer IZI, scientists using a similar technology were able to distinguish seven different bacterial strains.

At the same time, specially developed AI algorithms are expected to simplify the evaluation of VOC fingerprints. "Each measurement generates half a million readings", Schönfelder explains. "So we want to use machine learning to analyse this huge volume of data." The algorithm is trained using samples from healthy test subjects and cancer patients. The results of such measurements are available within a few minutes. "And we can well imagine that our ion-mobility spectrometer might one day be used to screen airline passengers so as to determine whether they are infected with the coronavirus", she adds.

Traceable measurements by atomic spectrometry

Mike Sargent
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The concept of traceable measurements is simple and well established.[1] Traceability solves the problem of ensuring that measurements of the same quantity are comparable even when made by different people, in different places or at different moments in time. Almost all measurements require a calibration of some kind. If measurements of the same quantity always use calibration standards derived ultimately from the same unique reference point, or primary standard, all will be based on the same measurement unit and hence comparable with each other. It is rarely possible to calibrate all measurements directly against the unique primary standard. The answer is a traceability "chain" comprising a series of calibrations using intermediate reference standards, the values and uncertainties of which are passed to the next link in the chain.

Provided that the measurement procedure is relatively straightforward, such as with everyday measurements of length and mass, comparability is sufficient to ensure consistent (or equivalent) measurement results. However, measurements such as amount of a chemical substance increase the complexity of the measurement procedure. In this case traceable calibration values will probably not be adequate on their own to achieve consistent results. Additional precautions such as formal method validation are then necessary. This applies to most measurements made by analytical chemists and is discussed later.

Global traceability

For a long time each community requiring traceable measurement results devised its own units and primary standards as well as the means to disseminate them. However, the 19th Century industrial revolution created the need for a single, global system. A convention held in Paris in 1875 resulted in an international treaty known as the Metre Convention.[2] The structure envisaged in the Metre Convention to support traceable measurements has continued into the 21st Century. Originally there were just three base units—for mass, length and time. Further base units were subsequently added and there are presently seven as shown in Table 1. These form the basis of the International System of Units, the SI.[3] More than seven units are in common use, but the others can be directly derived from those in the table. The most recent addition, in 1971, was the mole which is the base unit for the amount of a chemical substance. Until that point the Metre Convention was concerned solely with physical measurements.

Traceability in chemistry

Nevertheless, analytical chemists have become accustomed to using the physical measurement system because it underpins traceable calibrations for balances and volumetric glassware. This is important, but not an end in itself, because analytical chemistry is about more than determination of mass and volume *per se*; the analyst must measure the amount of the required element or compound. To achieve this, most instrumental methods require calibration of the instrument using solutions or solid artefacts containing known amounts of the target analyte. With direct analysis of solid samples the instrument response varies substantially with the overall composition. In this case reliable calibration requires the use of known values from "previously analysed materials" of very similar composition to the sample, i.e. matrix-matched reference materials. Both these and calibration solutions are chemical analysis standards

Table 1. The base units of the International System of Units (SI).

Physical quantity	Name of unit	Abbreviation
Mass	kilogram	kg
Length	metre	m
Time	second	s
Temperature	kelvin	K
Amount of substance	mole	mol
Electric current	ampere	A
Luminous intensity	candela	cd

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available from a wide variety of suppliers. However, for much of the 20th Century no attempt was made to apply the concept of traceability to ensure the consistency of their values. This was not feasible at the time due to the lack of a global chemical measurement infrastructure comparable to the physical one.

In the 1980s a move began to address numerous quality issues identified with chemical measurements. In particular, measurement laboratories were encouraged to seek accreditation to the ISO/IEC 17025 or ISO 15189 standards. Subsequently, this was extended to include accreditation of reference material producers to ISO 17034. Meeting the requirements of these standards for traceable chemical measurement results necessitated the creation of an appropriate international infrastructure. This was done by extending the one which had been developed for physical measurements over more than 100 years.[4] Calibrants with traceable values are now widely available, including many needed for applications of atomic spectrometry.

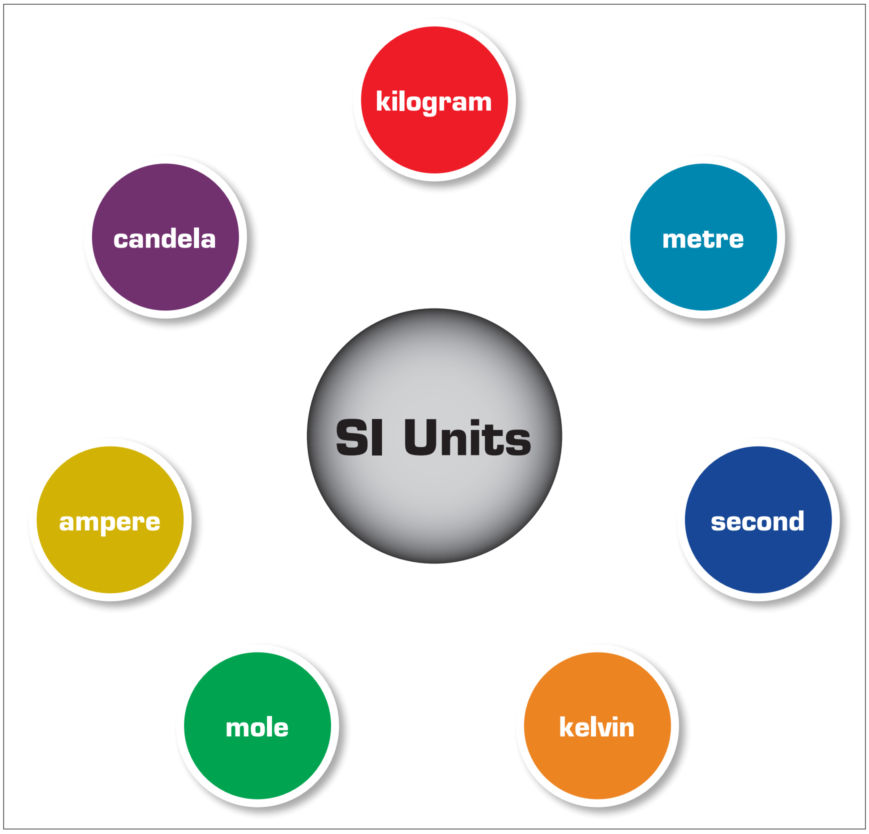
Making use of these materials requires laboratories to become the last link in the traceability chain. In addition to the chemical calibration standard or solution there will be another chain for calibration of the balance and perhaps also for volumetric glassware. Whether or not calibration values must be traceable depends on whether they contribute significantly to the overall uncertainty of the measurement result. Hence, matrix materials used for method validation should have traceable values. This is obvious if a matrix correction or recovery factor is subsequently applied to the results. However, even when a certified reference material (CRM) is used only to confirm 100 % recovery of analyte, the uncertainty of the certified value(s) still contributes to the overall uncertainty estimation for the measurement results.

Traceability in the laboratory

The tasks needed by the laboratory to take its place at the end of the traceability chain are straightforward, because they comprise best practice specified for laboratory accreditation. In summary, properly validate measurement procedures, estimate uncertainty and ensure full documentation. Calibration standards or matrix reference materials used in the procedure should have a traceability chain which is complete and fully documented. Commercial availability of suitable materials is generally good for many applications of atomic spectrometry. This is particularly true for most elemental analysis applications using techniques such as atomic absorption spectrometry, inductively coupled plasma-optical emission spectroscopy and inductively coupled plasma-mass spectrometry (ICP-MS) which are calibrated with single or multi-element solutions. Solid sampling techniques such as X-ray fluorescence or arc/spark optical emission spectroscopy are more difficult, due to the need for matrix-matched calibrations. However, older CRM stocks for applications such as steels, alloys and ores are steadily being replaced with modern materials having traceable values.

Wherever possible purchase commercial reference materials from a supplier accredited in accordance with ISO 17034. However, it is still prudent to carefully assess the materials. For example, ISO 17034 allows non-certified values to be included on a certificate. This is useful, but such values are unsuitable for calibration purposes and are unlikely to be covered by the certificate's traceability statement. There is no standard format for traceability statements and many are limited to unhelpful phrases such as "traceable to the SI".[5] Users should look for more detail, either in a more comprehensive statement or as additional information supplied with it. This usually includes the source of the traceable calibration values used in assigning values to the material.

Assignment of values to matrix reference materials often requires complicated methods and the producer should provide information about these, including how they were validated. Matrix reference materials values are frequently assigned by inter-laboratory comparisons. Claims such as "traceable to the methods used by the participants" are



unhelpful, so look for additional information. Materials with a very long shelf life, such as those used in metallurgy and geochemistry, also need caution. Many still on sale today were certified before current best practice using informal interlaboratory exercises, often without traceable calibrants. Moreover, these older materials may sometimes be used as calibration standards for certification of modern reference materials.

Traceability in practice

Sometimes traceable elemental calibration solutions are not available commercially or laboratories are not in a position to purchase them. Commercial solutions of analytes such as organo-metallic or isotopic materials are also less common. The laboratory then needs to prepare them in-house and assign traceable values. In principle this is not difficult and was once the norm for analytical laboratories. However, the devil lies in the detail. A common approach is to take a known mass of the analyte from a sample having known purity and dissolve it in a known mass or volume of solvent. Provided the balance and volumetric glassware have traceable calibration values the laboratory can demonstrate the traceability of the assigned value. The devil is the purity of the solid analyte sample. It does not necessarily need to be ultra pure, but the value assigned to the purity must be reliable and traceable. Ideally, the pure material should be a CRM but these are often unavailable. It is tempting to use commercial reagent grade materials instead, but these usually come with only an approximate estimate of purity or a batch specification. Such values are inappropriate for the preparation of calibration solutions. Some possible alternatives for three application areas are discussed below.

Elemental analysis

Unfortunately, few pure elements for preparation of calibration solutions are available as CRMs and undertaking a full assay procedure is not a trivial task.[6] However, many metals are widely available for other purposes in very high purity forms. These may be used provided suitable precautions are taken. A routine spectroscopic scan will confirm the absence of other elements even at trace levels. If impurities are identified at significant concentrations, it may be easier to find an alternative source rather than attempt to measure their amount accurately in order to apply a correction. In many cases, metals sold as "4 or 5 nines pure" are suitable but there are two potential problems. These metals may have pockets of occluded gases which could introduce an error in the calculated concentration of the solution. Some metals are prone to oxidation, producing a surface oxide layer and the surface should be cleaned before weighing them. Both errors can be reduced by using rod or wire instead of turnings or fine powders. It is also essential to ensure that metal is taken into solution quantitatively, which may not always be a trivial task.

Solutions of metals such as rhodium, which are available in high purity form but are difficult to dissolve, or of non-metallic elements, may be prepared from a suitable salt. However, dissolution of a known weight of the salt is rarely sufficiently accurate due to the lack of reliable data on stoichiometry, water content or impurities. The preferred option is to assay a solution of approximate concentration using a technique such as EDTA titrimetry. EDTA solutions with certified concentration are readily available or can be assayed using a certified solution of a metal such as silver. To ensure traceable results, each such calibration step must be accurate and its measurement uncertainty documented.

Speciation analysis

The hyphenation of ICP-MS with liquid or gas chromatography, or field-flow-fractionation allows analysis of organic compounds containing a metal atom or heteroatoms such as P and S. Used with appropriate analytes, this offers greater sensitivity than most conventional organic mass spectrometers and selectivity for molecules containing the target atom. It also allows an easier route to traceable measurement results than organic mass spectrometry. The latter also uses calibration solutions prepared by weighing analyte samples of known purity but there is a problem. Organic compounds close to 100 % pure are rarely available, so an accurate purity assessment is essential to avoid significant errors. This is not a trivial task[7] and presents major difficulties with large molecules.

There is, however, an alternative calibration approach for speciation applications using hyphenated ICP-MS. As the instrument response corresponds to the total amount of the metal or heteroatom, it can be calibrated using an inorganic solution of the target atom. Calibration solutions with traceable values are readily purchased or prepared as described for elemental analysis. This measurement does, of course, determine the total amount of the element and not the target organic molecule. However, the element-specific chromatogram will reveal the presence of any impurity peak(s) containing the target atom so a traceable value for the target molecule can be calculated. This approach has been used for compounds such as selenoproteins,[8] ferritin-bound iron[9] and carboplatin adducts.[10]

Isotopic analysis

It is sometimes forgotten that ICP-MS always makes isotopic measurements. A specific isotope of the target element is compared between the sample and calibrant solutions. This works provided the isotope's abundance is the same for both. Unless the element is mono isotopic there is no guarantee that this is true. For example, the natural isotopic abundance of lead varies quite widely and isotopic fractionation of some elements can be caused by processing techniques. Hence, to obtain traceable results it is necessary to determine the isotopic abundance of both the calibrant and the sample, applying a correction if necessary.

Calibration of mass spectrometry using isotope dilution analysis (IDMS) requires addition to the sample of an isotopically labelled material (the "spike"). This comprises, or is labelled with, an isotope having low abundance in the natural sample. Its ratio to a naturally abundant isotope is then determined. The popularity of IDMS calibration has increased with the wide use of ICP-MS,[11] but it is then essential to compensate for a variation in instrument response between the two isotopes, the so-called mass bias correction. Traceable values can be achieved by obtaining or preparing solutions of the isotopic spike with known amounts of the chosen isotope. An alternative approach is known as the "double" or "reverse" IDMS technique[12] which uses a calibration solution of the natural analyte. This requires a relatively complicated measurement procedure involving a sequence of "blends" in which both the sample and calibration solutions are spiked with the isotopic material.

Where next?

As we have seen, traceable results have a long and successful history with physical measurements. Fortunately, the global measurement infrastructure has now been extended to support traceable values in analytical chemistry. Hence, any spectrometry laboratory should be able to provide traceable measurement results by adopting current best practice. However, this depends on the availability of calibration standards and matrix reference materials with traceable values. Supply is already good for many elemental calibration solutions, but there is much more to do with matrix-matched standards. These are essential, for example, with the solid sampling techniques used in metallurgy and geochemistry. On the positive side, developing the chemical measurement infrastructure has encouraged many more national institutes to produce chemical standards and CRMs. These are available to laboratories but also provide the means for commercial producers to establish traceable values for their own products. Many of the national institutes also have active research programmes addressing traceability issues, including novel applications such as organo-metallics, protein analysis and isotopic measurements. Thus, we can be assured that traceable measurements in atomic spectrometry will have a long and successful future.

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analytica virtual 2020: a new platform in times of contact and travel restrictions

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2020 presented us, as a trade fair organiser, with major challenges to which we had to react to meet the demands of our partners and customers. In March it became clear that due to the corona pandemic the regular hosting of analytica at the originally scheduled date of late March/early April would be untenable. So, we decided to postpone the fair until October: a setback for our entire team. Up to then the trade fair had been heading for a new record, with more exhibitors than ever having already confirmed their participation.

However, it got worse! It soon became clear that visits to trade fairs for our European core markets would not be possible. A traditional fair under these conditions would have fallen far short of the requirements of the visitors and exhibitors. In early September, we, therefore, had to call off analytica in its usual format.

Fortunately, we had planned well ahead and in August we were able to launch the new analytica virtual format. Originally this was conceived "only" as a digital supplement to our existing physical formats in the global analytica network. However, in the end, analytica virtual, held from 19 to 23 October 2020, replaced the usual fair in Munich.

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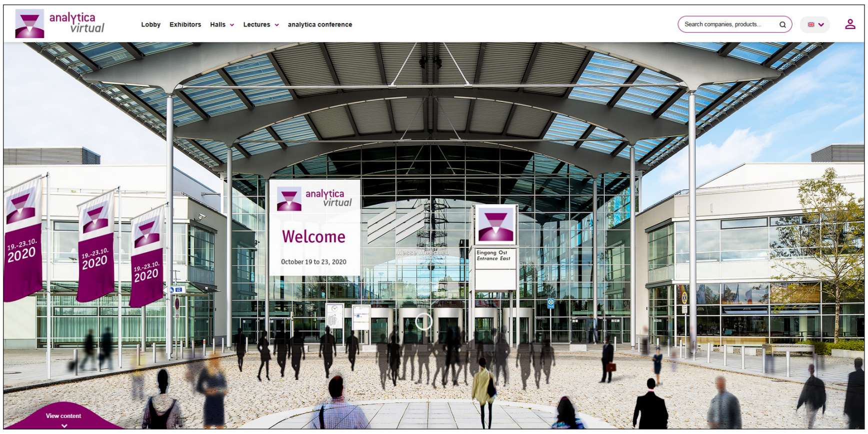


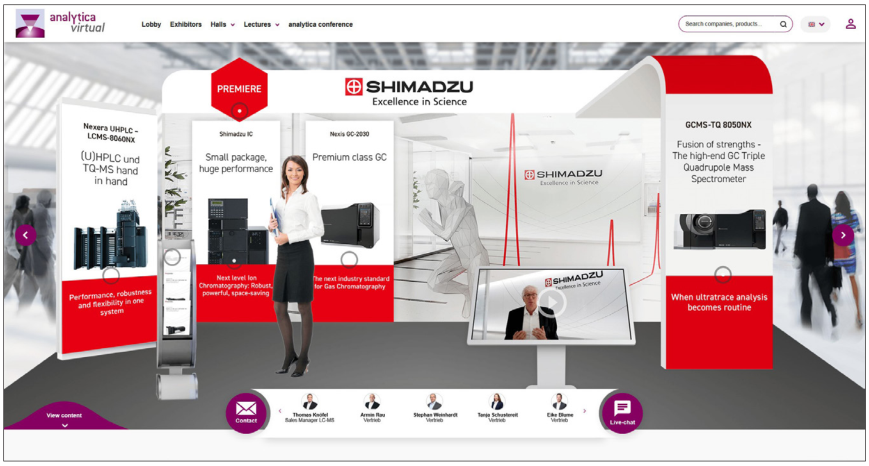
The entrance to analytica virtual: looks familiar?

The concept: online trade fair with virtual booths and supporting programme

Together with our partner, Lumitos AG, we managed to transfer as many of analytica's features as possible into cyberspace within the extremely short lead time. The conventional trade fair tour was replicated, with the improvement that the fair was open 24 hours a day. You could jump from one virtual booth to the next within a very short time and experience the digital product presentations of each. Based on positive customer experiences from previous virtual trade shows, we restricted digital product presentations to a maximum of four per virtual booth. This guaranteed the inclusion of only current and important innovations. Moreover, it did not overload the amount of information on the virtual booth and was easier for visitors to perceive. Exhibitors who wanted to show more innovations were able to expand their presence over several contiguous booths.

Replicating the traditional organisation of analytica, the booths were grouped into six virtual exhibition halls. These were dedicated to the areas of Premieres, Analysis & Measuring and Testing Technology, Laboratory Technology, Biotech & Bioanalysis, Diagnostics & Medicine, and Start-ups. Visitors could use search filters to narrow down exhibitors according to the main topics they were interested in. Communication between exhibitors and visitors took place via text, audio or video chat. In addition, visitors had the choice of 200 webinars from exhibitors.

Central elements of analytica's supporting programme were present in the virtual format as well. The analytica conference offered 119 specialist presentations connecting science and application—this time in the form of webinars.



A virtual booth.

The "Digital Transformation" special show presented eight exclusive digitised laboratory workflows in video demonstrations.

Participation in analytica virtual 2020 was free of charge for visitors.

Strong industry participation proves the relevance of the event

The efforts were worth it! All in all, a total of 21,641 participants (unique users) from 152 nations took part. 268 exhibitors from 24 countries presented more than 700 product highlights. There was a total of more than 33,000 participations in the 200 exhibitor webinars and the 119 scientific presentations at the analytica conference.

The 24-hour accessibility of the digital platform for easier global access proved worthwhile: analytica 2020 had the highest international share in its history. Half of the 21,641 participants (unique users) did not come from Germany. After Germany, most visitors came from Switzerland, USA, United Kingdom, Austria and India. Unsurprisingly, there was a strong influx of participants from Asia in the morning hours of Central European Time, while in the evening and night hours many Americans visited. On average, some 5000 participants attended the virtual analytica on each of the five days of the event—at peak times, it was over 7000.

We believe we succeeded in enabling the industry to present itself globally, 24 hours a day, despite the contact and travel restrictions. Visitors rated the virtual trade show, with its focus on new solutions and innovations, very positively. There were numerous repeat visits, webinars were strongly used, as were the facilities to download information and send enquiries to the exhibitors.

Start-ups, smaller and medium-sized companies, in particular, were pleasantly surprised by the internationality and the number of new contacts for products and webinars. Some exhibitors found that the quality of enquiries could not be compared with that of a classic trade fair. But the point was not to replace the strengths of a traditional trade fair.

The future of trade fairs, the future of analytica (virtual)

In spite of the success of the purely virtual held trade event, we still believe in traditional fairs. Especially in times like these, the importance of cultivating the human relationships which are the base for a successful business has become obvious. The personal contact, the random, spontaneous meetings and the detailed discussions that occur at a face-to-face event cannot be replaced. Detailed analysis, as well as the hands-on experience of products and solutions in need of explanation, also require physical meetings. This is also reflected by our exhibitors and partners. However, the virtual format presents opportunities to reach new interested parties all over the world! Budget and travel restrictions no longer play a role.

So, we are continuing to plan the next analytica in June 2022 on the fairgrounds of Munich. But we will also use the knowledge we have now gained to expand our range of additional digital offerings. Thus, the circle closes and we come back to our original planning, when analytica virtual was seen only as a digital extension of our proven existing fair formats.

Susanne Grödl has been Exhibition Director of the laboratory trade fair analytica in Munich since 2005. She also manages the international analytica network with trade fairs in China, India, Vietnam and South Africa. Previously, she worked for the information and telecommunications trade fair SYSTEMS.

Events, events!

…a perspective from the British Mass Spectrometry Society

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Harold Macmillan (British Prime Minister 1957–1963), when asked to name the most difficult thing about his job, responded (patricianly); *"events, dear boy, events!"*. The pandemic events of 2020 have had far reaching consequences for British Mass Spectrometry Society (BMSS) committee members both personally and professionally. In *Covidious Albion*, the BMSS's diary of scientific meetings was obliterated and we have all had to adapt to interacting via Zoom.

What are the realistic prospects for analogue scientific meetings in 2021?

The rollout of efficacious vaccines and the social imperative bodes well for the resumption of conventional meetings. However, the *unknown unknowns* of new COVID-19 variants coupled with the tightening of public and private sector budgets may allow only a modest revival of events in the latter half of this year.

"There are decades where nothing happens; and there are weeks where decades happen."[1] The COVID-19 rollercoaster, for the BMSS Events Team, began on 16 March 2020 with the first onset of lockdown in the UK. In the following months we all began to grasp the enormity of the situation, with the inevitable cancellation of a succession of one-day Special Interest Group (SIG) events and finally the abandonment of our financially critical three-day Annual Meeting scheduled for September 2020.

Since its foundation in 1964, the British Mass Spectrometry Society has progressively developed a programme of charitable disbursements. The Society's income and expenditure has for decades balanced on the knife-edge of a modest surplus generated from its traditional three-day Annual Meeting.

The BMSS took the view that its ethical response to COVID-19 should be to strive to keep the public discourse of mass spectrometry alive in the UK. The Society also thought it important to provide a platform for Early Career Researchers (ECRs) to present their work in the virtual space. Over the following months we collaborated with fantastic teams of SIG coordinators and sibling societies (e.g. the Mass Spectrometry Imaging Society) to deliver a programme of 26 on-line events to the mass spectrometry community at large.[2]

Going virtual has had significant benefits: we now have regular participants in our on-line events that range from Singapore in the east to Los Angeles in the west, from Auckland in the south to Stockholm in the north. We have made many new friends and they are a very welcome addition to the BMSS family. The downside is that, whilst we have made many new friends, we have struggled to develop an income stream to sustain the Society's charitable disbursements.

So, the critical challenge that faces many scientific societies in the short term is how to evolve a new funding model for the COVID-19 era that both serves the needs of members and delivers value to sponsors. We detect a marked resistance to charging delegates a significant fee for on-line events. We have all become accustomed to streaming unlimited entertainment (e.g. Netflix etc.) for a negligible monthly subscription, and that has set cultural expectations. We anticipate that inviting on-line delegates to make a donation (cf. the Wikipedia funding model) will only yield a very modest revenue and will not balance the books!

Feedback from our traditional sponsors (i.e. scientific instrument companies and scientific service providers) suggests that they are challenged to justify return on investment (ROI) when invited to support virtual events.

Will virtual events become adopted as the new normal?

In general, there is a human propensity to be wary of change. In this instance we think that that predilection will prevail, and that the overriding social imperative will triumph in the short term.

Necessity is the mother of invention! The pandemic has stimulated a multiplicity of innovations for the virtual hosting of major events (e.g. iVent,[3] vFairs[4] etc.). These solutions are fantastic but will not, in our opinion, replace the *roar of the bar and smell of the crowd*. We expect that

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the social imperative will prevail when public health restrictions abate, and so major traditional events will revive in the short to medium term.

The immediacy of personal interaction, the subtlety of subliminally observed body language and the sheer pleasure of doing business face-to-face will not be superseded by virtual conferencing in short order. So, the preferred option for major events will be *strictly analogue* in the foreseeable future.

Small virtual events (e.g. SIG meetings via Zoom), lasting no more than a couple of hours, have and are being adopted as positive enhancements to the scientific landscape and are likely to become enduring fixtures in our diaries long after the pandemic has been brought under control.

The roar of the bar and the smell of the crowd!

The social imperative impels us to seek out the company of our peers, to vigorously discuss our science face-to-face and engage in *networking events*. The desire of our community to resume traditional events, in the short term, is undeniable.

Simulating major events on-line, with current technology, has little traction with either prospective delegates or sponsors! Our members are resolute in their wish to see traditional analogue events revived. Our sponsors have made it clear that supporting virtual events is very hard for them to justify on the basis of ROI, …and we do not detect that that view is softening.

The BMSS conducted a member and community e-survey in March 2020: *Adapting to the Challenge*.[5] The objective was to gauge the community appetite for a virtual alternative to the Society's classic three-day Annual Meeting scheduled for September 2020. The results were illuminating; a small subset of enthusiastic members was very much in favour, the majority were agnostic and, most chillingly, the majority of the Society's sponsors and supporters were very sceptical. So, in light of the received feedback the Society elected to eschew a virtual alternate to its classic Annual Meeting in 2020.

Imagineering a low carbon event culture *ca* 2031

Project yourself forward a decade to a time where the internal combustion engine has become a relic, your home will be heated by a super-efficient heat pump, broadband of gargantuan bandwidth is universally available and carbon-hungry air travel will be déclassé.

In 2031, technology permitting, we may be able to readily engage in satisfyingly holistic and holographically virtual event experiences. The combination of most institutions' inclination to cut travel budgets (whenever a pretext arises), and the leading nations' stated intent to extinguish their carbon footprints may prefigure the twilight of the traditional international scientific meeting.

In 2031, only the elite of our community may be invited/permitted to travel (with appropriate carbon offsetting) to a glamorous location, conference with their peers and enjoy a tincture on the terrace before a terroir-specific dinner.

The privilege of encountering new science/colleagues/places/cultures/foods at first hand (that was part and parcel of the traditional ECR's professional trajectory) may become the preserve of a very select few. This may have implications for social mobility and professional inclusion for a generation or more. We may see the emergence of a patrician old guard (underpinned by personal networks formed on the traces of grand hôtels in times past) competing with a younger and *strictly virtual* cohort. In the long term everything will come into equilibrium, in the medium term it may spawn a decade or more of unintended *segmentation*.

Come fly with us…

Attendance at international conferences (e.g. ASMS, IMSC etc.) has become part of our community's culture. As we all know, in response to the pandemic, most major airlines have mothballed or scrapped significant portions of their fleets (British Airway's *Queen of the Skies* 747-400, for example). The rollout of viable vaccines may well open the door to a renewed freedom to travel, and so unleash pent-up demand to do so! It is possible that demand for seats my outstrip supply in the second half of 2021 and so ticket prices may be expected to rise.

The BMSS, and analogous societies, have established programmes to provide assistance to their members (typically ECRs) to facilitate their participation at international conferences. The projected increase in the price of air travel in the second half of 2021 combined with the paucity of charitable income in 2020 presents a cash flow challenge that we have all yet to rationalise.

Looking to the immediate future with pragmatic realism

Reviving traditional scientific events, within 2021, is fraught with challenges! The rollout of efficacious COVID-19 vaccines is fantastic news—however, that will not solve the scientific event organisers' challenge in 2021! Academic and corporate travel policies (and marketing budgets) were crystallised around the fourth quarter of 2020. Coming off the back of a tough year in 2020, budgets have been cut to the bone, and so prospective delegates and sponsors will be very hard to secure.

Being pragmatic, the BMSS will revive its Annual Meeting when circumstances permit. We are aggressively researching a modest 1.5-day event for September 2021 as a stepping-stone to a classic three-day meeting in 2022. The BMSS is most grateful to its members and sponsors for encouraging the Society on that challenging journey.

The path to reviving analogue scientific events in 2021 will be turbulent! The organisers involved may rationalise their experiences *post facto* as a rite of passage,

…fasten your seatbelts it's going to be a bumpy right!

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Mark is the Meetings Secretary of the British Mass Spectrometry Society and a Trustee of the BMSS. Prior to retirement he held senior management roles in applications development, scientific marketing and business development at Waters Corporation, Micromass UK Limited and VG Instruments.

DIARY

Conferences

2021

15–20 February, Houston, United States. **2021 AAFS 73rd Annual Scientific Meeting.** 🕸 https://www.aafs.org/aafs/Meetings/2021-AAFS-Annual-Scientific-Meeting/AAFS/Meetings/2021-Meeting/2021-Annual-Meeting.aspx

18 February , Online. **February Meeting of the New York Section of SAS.** https://www.spectroscopyeurope.com/events/february-meeting-new-york-section-sas

7–11 March, New Orleans, LA, United States. **Pittcon 2021: Conference on Analytical Chemistry and Applied Spectroscopy.** ✉ pittconinfo@pittcon.org, 🕸 https://pittcon.org

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

1–3 June, Kristiansand, Norway. **10th World Conference on Sampling and Blending (WCSB10).** ✉ contact@wcsb10.com, 🕸 https://wcsb10.com

1 June–31 July, Denmark. **International Association for Spectral Imaging (IASIM).** ✉ 2020@iasim.net, 🕸 https://2020.iasim.net

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

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

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

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

2023

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

Exhibitions

2021

23–25 September, Hyderabad, India. **analtytica 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

Letter to the Editor: origins of volume fraction for better calibrations

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A couple of columns ago we reported on work which had shown that weight fractions were often incorrect concentration units to use in quantitative chemometric studies.[1] The article prompted some interesting feedback, not least a long "Letter to the Editor" from the originator of these ideas. His own work proving the importance of using volume fraction not weight fraction when the samples are made up of liquids of different densities had struggled to be published in chemistry journals. I was pleased that Howard had reached out to us from across the Atlantic, especially at a time of great upheaval in the USA, and with Ian Michael's approval we have decided to feature Howard's letter in this month's column as it also sets straight a few misconceptions that were in our original look at this problem. So over to Howard!

Letter to the Editor—Howard Mark

Your column was a very nice review of the current status of investigations into the nature of "concentration" for spectroscopic analysis. I already knew about the "Mythbusters" article and some of the other articles you mention. But two are new to me: I had not previously heard of the work by Yan *et al.* and by the Analytical Methods Committee.[2–3] So I want to thank you for bringing them to my attention.

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To be sure, when wet chemistry was the premier method of chemical analysis, weight% was the natural, and indeed the best, basis for the analysis. It was the easiest, as well as the most precise and accurate, technology available to use; a standard analytical balance could weigh 100 g to 0.1 mg: 1 part in a million precision. It could be standardised by subjecting a specimen of pure analyte to the same analytical procedure used for "unknown" samples. Even nominally volumetric methods of analysis were usually converted to a weight basis for reporting. I never did that commercially, but when I was in school, "Analytical Chemistry" meant gravimetric and volumetric analysis.

So, it was always natural to use those gravimetric results as the "reference laboratory" values for spectroscopic analyses. Nobody thought there could be a problem aside from bad lab technique [key in "bad lab values" as one of the major problems for near infrared (NIR) spectroscopy]. Even when I had general thoughts to consider nonlinearity effects on spectral results, I did not think how it would apply to the specific problems we had in understanding NIR spectra, or even that it could apply as described.[4]

"Mystery" non-linear phenomena?

I did, however, always have a nagging feeling in the back of my mind that some of the unexplainable phenomena we observe in calibrating for quantitative analysis using NIR spectra could be explained by invoking some "mystery" non-linear phenomenon. However, I had no clue, any more than anyone else, what the cause of that mystery could be—it was a mystery!

Everyone looked at the instruments, but the engineers did wonders in keeping non-linear effects out of the instruments, and any that remained were well-explained by known optical phenomena in the sources, optics, detectors and even the samples. Furthermore, there was never evidence for any of the effects I described in 1988 being present in analytical data. Sample effects were known [log (1/*R*)?, Kubelka–Munk? etc.) but calculations and experiments to elucidate these always gave the wrong order of magnitude to explain them.

The whole thing remained a mystery until I got a group together to do what amounted, almost by happenstance, to be the critical experiment that resolved the mystery. I didn't expect that. My goal at that time was not to do any "great science" or even look for anything new. It was intended to be a tutorial, to use and explain and describe the classical least squares (CLS) algorithm. In fact, the work described in the 2010 *Applied Spectroscopy* paper[5] was not the first time I tried it. I had previously done a similar experiment using water, ethanol and ethanoic acid. Those results were never formally published, but did see daylight in one of our columns.[6] In fact, that whole set of columns and my textbook with Jerome Workman comprise a superset of information about the experiment and about my thoughts while figuring it all out.[7,8]

Severe spectral distortions due to interactions between mixture components

When using CLS, the "validation" step comprises predicting the spectrum of the mixture, and with a whole set of spectra, the spectra of the components of the mixture. Using water, ethanol and ethanoic acid to make up mixtures, the distortions of the spectra of the components are so severe that there Is no question that interactions are playing havoc with the results; there was no need to speculate about that. Dumb me: I should have known that, but I have been so far from chemistry, for so long that I forgot about hydrogen bonding!

However, as a tutorial about CLS, it was straightforward to set up an experiment that would minimise or eliminate all the known or suspected sources of error in NIR spectroscopy:

- Using clear miscible liquids removed effects due to optical scattering and inhomogeneity
- Measuring transmittance meant that Beer's Law was the theoretically correct data treatment
- Mixture ingredients were all pure liquid hydrocarbons that should not interact [I wanted to use CCl_4 (carbon tetrachloride) but good sense prevailed and we used methylene chloride and chloroform instead].

The ingredients were measured out gravimetrically, so there was essentially no error in knowing what was in the mixtures; importantly, there was no (conventional) "reference lab error".

Fortunately, CLS was already preselected as the calibration algorithm, and it had the additional benefit of not requiring any user input of parameters, such as number of factors or number of wavelengths eliminating the risk of "over-fitting".

So, the experimental design was set, and (also importantly) there was no room for fudging the hardware, software or calibration. It was for a tutorial example, so it HAD to work! Nothing could go wrong…

Hydrogen bonding eliminated as a source of error, however…

Imagine my shock when I saw as much as 20–25% discrepancies between the spectroscopically measured values and the precisely known amounts of the ingredients!

Of course, the first thing we checked was the execution of the experiment, of which the first one was carried out by Ron Rubinovitz, a Senior Applications Scientist at Thermo Fisher Scientific. I told him about my results, we discussed the possibilities for errors in the experiment. Ron is a smart guy and a good experimentalist. He was able to convince me that he had all the potential experimental problems covered: I don't even recall all the things he checked for, but I remember the precautions he took, for example, to prevent evaporation, and checking against that possibility by weighing the cell before and after making the optical measurements; also weighing the cell statically over (relatively) long periods of time to verify its integrity and freedom from leaks.

At that point my mind kept going round and round trying to figure out what could be wrong. Could it be the spectral measurements? No, the CLS algorithm was able to reconstruct the spectra of the mixtures very well. Could the computer be acting up and giving wrong answers? No, there was more than one computer used and they agreed on the results. Besides, when a computer goes bad, it does not just make small errors, the whole thing fails to work. The only thing not accounted for was the reference values, could that be it? No, I've already justified the precision and accuracy of the reference data. Everything was working properly—except the experiment! The mystery was showing its head.

Eliminating all other sources of error pointed to the wrong reference concentration values

With experimental errors eliminated, I had to believe that the spectroscopic values were correct. So, eventually, I narrowed it down to the question of were these the right reference values? Normally, when we apply chemometric algorithms, one of their properties touted is the way they automatically include any necessary scaling factors. But CLS doesn't do that; recall "… there was no room to fudge the calibration"; CLS is the nearest thing we have to an "absolute" measurement method in spectroscopy. So that pointed the finger at not using the correct values to compare the calibration against.

But what, then, were the correct values? I had no idea. But I took it as a given that there had to be SOME physical property that was related to the absorption, otherwise all that I learned about science was out the window, and MAGIC was back in. By then all I could do was to generate other values, using known physics and chemistry to try out what could be correct.

Essentially the Edisonian approach; the details are in the *Applied Spectroscopy* paper.[5] What gratified me most about tracking down the source of these discrepancies was that ever since I got involved with NIR spectroscopy, the technology, useful and important as it is, always seemed to exist in a universe of its own, separated from the rest of the scientific universe, and connected to it only by bunch of arcane mathematical formulae. As a scientist I knew there had to be more, but until I comprehended the results of this experiment, I could not figure out what that was.

After the (mental) dust settled I told Don Dahm (author of *Interpreting Diffuse Reflectance and Transmittance: A Theoretical Introduction to Absorption Spectra of Scattering Materials*) about my results and asked him what he thought.[9] His response was "well, every physicist knows that!" Later I spoke to other physicists, who agreed with and even reinforced Don's comments. It seems that Maxwell's equations, the fundamental equations of electromagnetism that describe all the classical (i.e., pre-quantum mechanics) properties of light, are all derived on the basis of volume effects. Every physicist knows that! Here is the connection between NIR and the rest of the scientific universe. But that information never seemed to have made it to the chemists.

And the reason I'm writing at such length, is to correct misconceptions that always seem to creep into discussions about NIR spectroscopy. It seems that even chemometricians, who should know better, are subject to them, let alone chemists, who can be forgiven for them but who should still be corrected.

How errors enter chemometric equations

One primary issue is how errors enter into the chemometric equations. When Gauss derived his equations showing that Least Squares regression gave the same results as Maximum Likelihood calculations (which were the way relations between experimental data had previously been related), he also placed certain restrictions on how the data were to be handled. He specified that any errors affecting the relationship between the X (independent) variables and the Y (dependent) variable had to all be in the Y variable. The X variables should all be error-free. Modern discussions (e.g., my favourite book on the topic: Draper and Smith's *Applied Regression Analysis*) of the topic analyse the effects of failing to adhere to Gauss' prescriptions. It is not pretty.[10]

So, when I read your article, I could not help but note some misconceptions that continue to be promulgated. One of these is "The Great Mystery" of spectroscopy: why do quantitative spectroscopic measures of concentration go non-linear at higher concentrations? The answer to that question was immediately clear once I understood the results of my experiment. If two variables (weight fraction and volume fraction, in this case) are non-linear with respect to each other, then they cannot both be linearly related to any third variable.

Historically, quantitative analysis by wet chemistry was agnostic to the nature of the "reference value" because the reference standards used the same units as the samples. As discussed above, however, weight percents (or weight fractions) were overwhelmingly used in NIR analysis. But we were suddenly comparing those gravimetric measurements to a technology that was NOT agnostic, but had a built-in physics that required an inherently volume-based measurement (i.e., volume fractions).This made it clear to me that volume fractions were the "concentration" measure to use. This is irrespective of whether it "improves" calibration properties or not, it is still the correct units to express analyte concentrations in.

Above, I mentioned the separation of NIR analysis from the mainstream of scientific thought and effort. In particular, NIR spectroscopy has not conformed to the standard theoretical background that modern science is based on.

One other major misconception I found in your paper was where you stated "Howard selected CLS for his study, partly because it is the easiest chemometric model to explain…" While strictly speaking, saying that "CLS … is the easiest chemometric model to explain" is a true statement; but that was NOT the reason I chose to use it.

The reason I chose CLS was because I wanted the experiment to conform to the limits of the physics involved, and not be "improved" (or disimproved) by the user's choices. This way, it comprised a test of the conformance of NIR analysis technology to the rest of the universe of standard physics and science; then the discrepancies could point me in the right direction.

For say, 40 of the 45 years I've been concerned with NIR spectroscopy, I've been seeking the point of connection, so conducting an experiment where only the fundamental physical limits affected the results and the conformance of the NIR method to the rest of known science gave me confirmation that I was on the right track. I had little interest in producing the "best" calibration (in conventional terms of the Standard Error of Prediction or SEP); rather I wanted to gain understanding of how NIR spectroscopy works, as a piece of the scientific universe.

The world (and especially the NIR community) does not understand that approach. I have had papers rejected because I didn't compute an SEP. Clearly the reviewers had no clue as to what was actually going on, "if it's NIR there must be an SEP" was all that mattered in their world. I could have computed an SEP, which would have been a numerical measure of how well the CLS algorithm was "predicting" the pure ingredient spectra. The value of SEP would have been on the order of 10^{-4} to 10^{-5}, but that number would have been meaningless in terms of any real knowledge about either NIR spectroscopy or its ability to perform analysis. A nice test of the CLS algorithm, though!

So, I seem to have run on at some length, and I'm not entirely sure what it's all saying. So, let me just thank you again for publishing that review.

Conclusions

First of all, many thanks to Howard for explain much more deeply the history of this issue and his more thorough approach to reaching his conclusions… I'm very pleased we didn't get too much wrong (!). And I want to thank Ian and Tony for affording me so much space to explain the meaning of those experimental results, and hope that other scientists can pick up the ball of Science and run with it, without being distracted by mathematics (important as it may be).

Everyone please, stay safe!

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After receiving the PhD degree from New York University, I got my first exposure to NIR when I joined Technicon Instrument Corp. in 1976. That was shortly after Karl Norris developed and made public his new technology, based on the use of the NIR spectral region, combined with reflectance measurements and computerised data analysis to extract the information contained in the data. I've been trying to understand how and why it works, ever since! After Technicon closed down, Howard became a consultant for the NIR industry, assisting in both instrument development and rendering applications assistance. He also wrote several books related to NIR and calibration development: *Statistics in Spectroscopy*, *Principles and Practice of Spectroscopic Calibration*, *Chemometrics in Spectroscopy* (Edns 1 & 2) as well as contributing several chapters to all four editions (4th Edn in press) of *The Handbook of Near-Infrared Analysis*.

A new quality challenge

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Every now and then a new analytical challenge appears and, for the most part, the ISO/IEC 17000 series of standards adapts and evolves to include the new challenge. The latest challenge, testing for the presence, or absence, of the virus that causes COVID-19 seems to be a particularly difficult challenge.

How can this be? It is worth first looking at how chemical and clinical metrology has evolved over the last 25 years since I became part of this never-ending journey. On my journey I have learnt some basic truths about analytical science and how quality, reliable data can be developed, mainly through the application of ISO/IEC Standards.

The publication of ISO/IEC 17025 in 1999 was the genesis of robust quality management in analytical science. The standard requires, amongst many other things, validation of the method used, in some cases including sample collection and preparation where this part of the analytical process has a significant impact on the final result. Instrument calibration follows, using wherever possible Certified Reference Materials (CRMs) produced by an ISO/IEC 17034 accredited producer and on-going quality control using Reference Materials (RMs). Periodic proficiency testing is also required, if available, from a provider accredited to ISO/IEC 17043.

The application of the 17000 series of ISO/IEC Standards to chemical metrology differentiates it from many other areas of scientific measurement, in that unlike most ISO standards for management systems, assessment of the laboratory is normally carried out by a third party, normally the national organisation responsible for accreditation. Laboratories are, therefore, "accredited" under ISO/IEC 17025, rather than "certified" or "registered" by a third-party service as is the case with ISO/IEC 9000 quality standard. The Accreditation Body attests annually the technical competence within a laboratory, in addition to its adherence and operation under a documented quality system, specific to a Scope of Accreditation.

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The result of this is that the quality of analytical data produced by ISO/IEC 17025 accredited testing laboratories in the environmental, food and beverage, pharmaceutical, minerology and metallurgy and construction materials sectors has reached a level of excellence which means the original concept behind ISO/IEC 17025, "Tested Once, Accepted Everywhere", is slowly becoming a reality in many sectors. There are concerns: many respected scientists would never employ any analytical lab without independently reassuring themselves of the lab's competence. Experience shows it is possible to send the same sample to three accredited labs and get three significantly different results.

One of the features of the ISO/IEC 17000 quality management umbrella is that the product of testing, analytical data, should wherever possible be accompanied by an estimate of total uncertainty and traceability to the SI system, through an unbroken chain of comparisons.

In clinical chemistry the basic tenets of the ISO/IEC 17000 series approach to quality management have been included in ISO/IEC 15189, which is, in effect, the Accreditation Standard for medical and diagnostic testing. In validating a diagnostic or clinical test, the Sample Preparation and Extraction or Sample Preparation stage would always be also validated, since recovery from the bio matrix varies significantly from method to method.

Also, as I understand it, ISO/IEC 15189 applies to all clinical tests, "where appropriate" including small molecule, drug or endogenous small molecules used as bio markers. The main reason that large molecules are not included, be they proteins or oligonucleotides, was that CRMs or RMs have not been routinely available and that there is difficulty in linking chemical amount of substance with biological activity. So, it is very difficult, or impossible, to demonstrate commutability, which is defined as "the equivalence of the mathematical relationships between the results of different measurement procedures for a reference material and for representative samples from healthy and diseased individuals".

This brings me to the tests used to detect infection from the COVID-19 virus during the present pandemic. Polymerase Chain Reaction (PCR) tests are nothing new; they were first described in 1983 by the American biochemist Dr Kary Mullis at Cetus Corporation, and for which he won a half share in the 1993 Nobel Prize for inventing the PCR process.

Since then, PCR tests have been used to measure the presence of DNA, especially in forensic analysis and the study of DNA in research applications. Most PCR methods utilise thermal cycling; this exposes reactants to repeated cycles of heating and cooling to allow different temperature-dependent reactions, primarily DNA melting and enzyme-driven DNA replication. PCR employs two main reagents—primers (which are short, single-strand DNA fragments known as oligonucleotides that are a complementary sequence to the target DNA region) and a DNA polymerase. In the first step of PCR, the two strands of the

DNA double helix are physically separated at a high temperature in a process called nucleic acid denaturation. In the second step, the temperature is reduced so the primers bind to the complementary sequences of DNA. The two DNA strands then become templates for DNA polymerase to enzymatically assemble a new DNA strand from free nucleotides, the building blocks of DNA. As PCR progresses, the DNA generated is itself used as a template for replication, setting in motion a chain reaction in which the original DNA template is exponentially amplified. The formula used to calculate the number of DNA copies formed after a given number of cycles is 2^n, where n is the number of cycles. Cycling continues until a fluorescent indicator included in the reagents binds to the synthetic DNA and can be detected. Thus, a reaction set for 30 cycles results in 2^{30}, or 1,073,741,824, copies of the original double-stranded DNA target region.

It must not be forgotten that the higher the number of cycles needed to reach a detectable signal for the viral genome, the lower the amount of viral load that is in the sample; the lower the number of cycles, the more prevalent the virus was in the original sample. It would be helpful if the number of cycle thresholds needed could be used as an important metric by which patients, the public and policy-makers can make more informed decisions about how infectious and/or sick an individual with a positive COVID-19 test might be, but there is absolutely no evidence to support such an assertion.

A recent study from the Infectious Diseases Society of America,[1] suggested that at 25 cycles of amplification, 70 % of PCR test "positives" are not "cases", since the virus cannot be cultured because it is dead, and by 35 cycles it is reported that 97 % of the positives are non-clinical. The study has not been validated by others and it is worth considering that without evidence linking the data to clinical histories it is possible that the "false positives" may be because the virus has been cleared from the body by the patient's immune system, leaving unviable RNA fragments.

As stated above, rt-PCR is not testing for disease, it is testing for a specific RNA and this is the key pivot. At 25 thermal cycles, 70 % of the positive results are not really "positives" in any clinical sense, since fragments of RNA cannot make anyone ill. Further, it is the functioning of complete viral RNA inside the infected cell that does lead directly to making a person ill, so this diagnostic assay is not detecting infectious virus but solely the viral genome.

Despite not being intended as a diagnostic tool, developments in PCR have made possible the rapid and highly specific diagnosis of certain infectious diseases, including those caused by bacteria or viruses. Cai *et al.*'s paper[2] explains this in more detail, from a medical perspective.

Viruses are unique in having a genome composed of either DNA or RNA and unlike every other "living thing", never both. There are, however, many viruses whose genome is composed of DNA, good examples are *Varicella zoster* (chickenpox), herpes simplex etc. There are also viruses, e.g. HIV, that have an RNA genome in the virus, but which generate a DNA copy of their genome as part of their replication process. The SARS viruses are all RNA and the first successful use of Reverse Transcriptase PCR (rt-PCR) was with the development and validation of a method to detect the SARS-CoV-2 viral genome.[3]

It is hardly surprising that rt-PCR was the method of choice to detect the COVID-19 as it is a member of the same SARS-CoV-2 family of viruses, along with at least four common cold viruses. The development of a COVID-19 diagnostic test was carried out at great speed by a multitude of teams, all based on the genome released by the Chinese researchers in January 2020. An article by Vandenburg *et al.*[4] noted that more than 260 different rt-PCR tests for COVID-19 had been developed.

Vandenberg *et al.* also pointed out that the new, novel rt-PCR tests are not yet fully validated and should be considered as simply qualitative tests. There are most certainly grounds to believe the tests produce false negative results, as Kucirka *et al.*[5] make clear.

Applying an ISO/IEC perspective to all of this suggests that, whilst further optimisation of tests and more extensive clinical and epidemiological validation, including formal FDA/EMEA approval, are still needed, an ISO/IEC Standard that can be used when developing future new novel test methods is also needed. The lack of rigorous method validation and appropriate Quality Assurance/Quality Control (QA/QC) leads me to three real concerns.

Sampling

Taking a swab from specific areas at the back of the throat and upper nose is not simple: to take samples effectively and reproducibly requires the sampling procedure to be standardised and carried out by trained personnel, yet many samples are taken at home by the patient or a patient's family member. This adds a significant potential for error through incomplete sampling.

False positives

All the PCR tests are based on detecting a specific fragment of viral RNA. So, they all amplify sequences from two viral genes (ORF1a, or viral spike protein, that is the gene used for vaccine development and the N, or nucleocapsid, gene) and a positive PCR signal is required for both genes before the test is scored as positive.

Without a standardised viral fragment to be used for both target and as a reference sample and without real agreement on the number of thermal cycles, effectively setting a detection limit, the rt-PCR test remains but a qualitative screening test and not a diagnostic tool.

Commutability

A fragment of RNA found in a nasal swab can have three possible sources. Infected cells shedding active viruses, remains of dead viruses killed by the host's immune system (these can linger for weeks or months after the patient has recovered from the infection) and dead RNA fragments inhaled from the environment. Only infected cells shedding active viruses are of medical or epidemiological concern, dead viruses are background noise. Jaafar *et al.*[1] have demonstrated that many positive tests are from non-viable RNA, and so cannot be grown using classical virology methods: in a way this is a demonstration of negative commutability.

In mid-December 2020 the WHO issued guidance[6] on the use of rt-PCR as a diagnostic tool for COVID-19, warning users that any positive result (SARS-CoV-2 detected) or negative results (SARS-CoV-2 not detected) should not be used in isolation but in combination with specimen type, clinical observations, patient history and epidemiological information.

There are research efforts to find other ways to detect viruses: Professor Christelle Prinz and Dr Edouard Berrocal working at Lund University in Sweden[7] have been funded by the European Research Council to further develop a novel spectrophotometric method for the measurement of viruses. The article is interesting, and could be a significant new development, but the question of commutability still remains. The lateral flow test has attracted much attention; unlike PCR, it does not test for viral RNA but particular proteins made by the virus. Instead of taking two days to get a result, they take half an hour or so.

Taken together these issues show that the present testing regime in many countries fails to meet the requirements of ISO/IEC 17025 or ISO/IEC 15189 and Good Laboratory Practice. I do not believe the rt-PCR tests as presently used for mass testing can be considered to be any more than a qualitative screen with a high level of uncertainty, and should only be used along with other methods and a classical review of demonstrated symptoms to confirm infection of symptomatic patients. Despite this, various Governments believe their response to the pandemic has been science led, when in fact the opinions of a few notable high-profile scientists interpreting a test that is not proven to be fit for purpose as a diagnostic tool has been the main driver.

Why do I hold this view? Back in the early 70s, during my second year at Brunel University, we had one-term course entitled "Fundamentals of Science", given by Dr John Dore, a botanist. The takeaway message from the course was that as a scientist you have to question everything you read or are told and trust nothing that has not been third-party verified, if possible, by someone you know and trust. I think this is a principle that applies to everything that is described as "science" and made public in any vehicle. I have stuck to this approach throughout my career.

Although I started out my postgraduate career as a medical biochemist, studying at the Woolfson Centre at Birmingham University under Professor T.P. Whitehead, one of the "founding fathers" of external Quality Assessment of Clinical Laboratories, I migrated quite quickly into the commercial side of analytical chemistry and biochemistry, including microbiology. So, I do have the background to be able to take an objective view of what is happening.

I am profoundly unhappy that many Governments are making changes to society that impact on the life and health of many using data from a qualitative test that has a high level of uncertainty, caused by sampling error, lack of method validation and no real QA. It is simply bad science and undermines public trust in "science".

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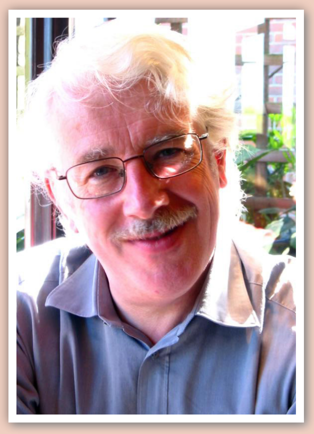

Since graduating from Brunel University London in the mid-1970s, I have been closely involved in the building of Quality Business in Analytical Science around the world. It has been a fascinating and enjoyable journey through the ever-changing analytical chemistry world. I've had to constantly seek out new developments and opportunities, technical, commercial and geographical. In 2013, I was invited to become a Fellow of the Royal Society of Chemistry, in recognition of my contribution to increasing awareness of metrology in chemical analysis. I have held senior roles in business development and licensing for a number of manufacturers.

Quality Management: the heart of the Quality Assurance/Quality Control process

Oscar Dominguez
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Business decisions in society and across a wide swath of industry sectors are often data-driven, making sampling reliability and analytical data quality of paramount importance. Quality Management (QM) plays a vital role in the Quality Assurance/Quality Control process. Oscar Dominquez here presents the critical role of QM in the mining sector, where everything is BIG: tonnages, challenges, environmental impact, profits, risks—illustrating how proper sampling is a major critical success factor also here. But the mining sector view is not unique; the QM prerogatives can be carried over to very many other sectors as well.

Mining: where everything is BIG

In the mining sector, decisions and investments in exploration, infrastructure construction, mining operations, ore processing and transportation require multi-million dollar capital and operating budgets, but critical decisions can be based only on very small samples (of the order of a few grams) that are *supposed* to represent thousands of tons. It is clear that the compound, complex lot-to-analysis pathway must be representative in all stages, Figure 1. The Theory of Sampling (TOS) is a self-evident element in the full Quality Management (QM) scope.

This was one of the most influential observations that led Pierre Gy to develop the TOS and later led researchers such as Dominique Francois-Bongarcon and Francis Pitard, among others, to promote, convince, quantify and demonstrate to executives and mining professionals the severe risks to which businesses expose themselves should they compromise sample quality in a misguided attempt to reduce costs. Over many decades, examples of this practice have been accumulating, but not many have been published (for obvious reasons). It will suffice to refer to two major communications from the sampling world.[1,2]

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In this context, supervisory programmes have been developed to establish Quality Assurance/Quality Control (QA/QC) parameters that monitor correct execution of sampling protocols and control each stage of the "sampling cycle" [sample collection, preparation and analysis (method)] to preserve, quantify and ensure sample representativity, Figure 2.

QA/QC reports commonly include statistical–numerical results that quantify performance of QA/QC controls (field duplicates, preparation duplicates, blanks, standards etc.). Graphics such as scatter plots, QQ plots, histograms and cumulative frequencies are used to represent the results graphically. Statistical values normally include, for example, relative differences, absolute differences, relative variance, averages, T-test and Z-scores, which are used to quantitatively express the relationship between duplicate pairs… However, is an effective quality programme simply just a statistical exercise? And will pairwise comparisons be able to detect all possible wrongdoings (especially be able to detect a sampling bias)?

The following discussion considers these questions in the context of a *quality programme standard* as outlined by the JORC code (http://jorc.org), that is intended to highlight and emphasise a call to return to basics during this era of new technological applications and advanced statistical analysis.

The case for proactivity

This paper aims to highlight the concept of "QM" as the precursor for appropriate corrective actions to close gaps determined by the execution of a quality programme, specifically *trend analysis* (by ranges time and/or grades), with the aim of proactively determining control

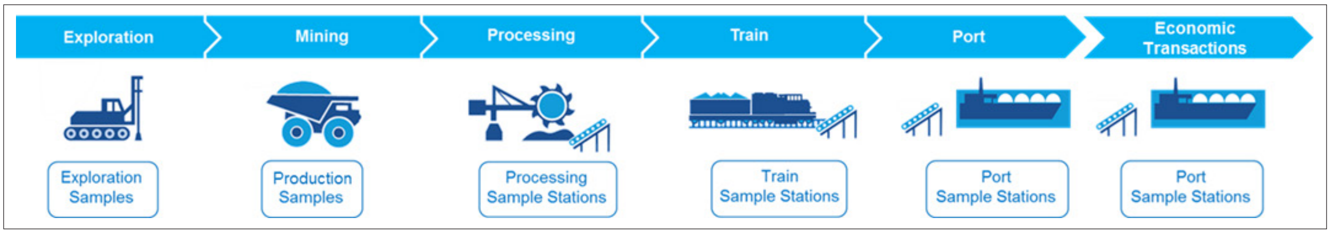


Figure 1. The mining value chain. Rectangles indicates where samples (and their analytical results) are used to support critical business decisions.

performance deviation and thus proactively rectify the source of deviation.

Sometimes, there is confusion among those accountable for QA, and even among auditors, that if individual data points fall within predetermined acceptance limits, they are then necessarily acceptable and, therefore, suitable as a basis for operational and investment decisions. A similar situation is that tabular statistical summaries are enough to demonstrate acceptability of QC outcomes. However, what is stated with respect to QM is that sometimes results found within the acceptance limits can be *de facto* **internally biased**, or show material deviations over a period of time, thereby still impacting operational performance. An unstable process which happens to plot within acceptance limits for some restricted time interval is nevertheless an unstable process at large. Thus, true process control requires something more.

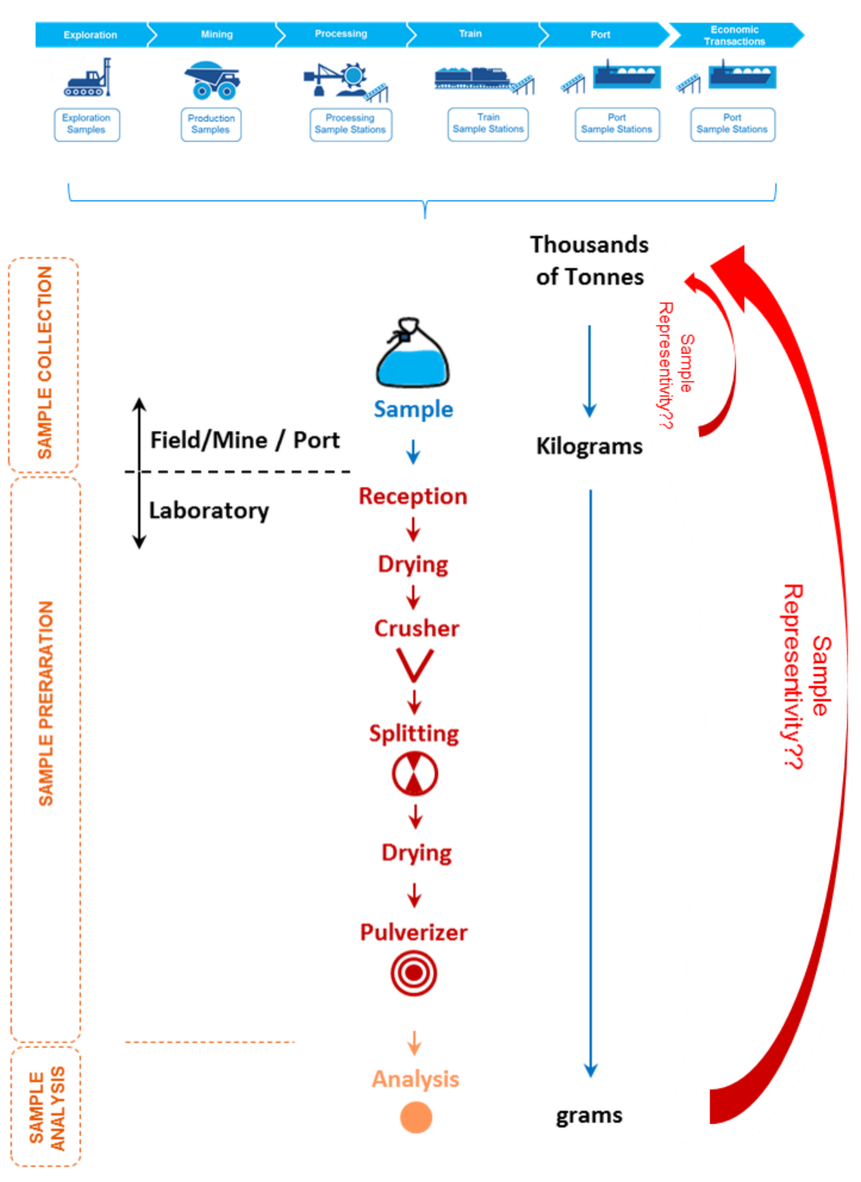


Figure 2. Schematic diagram showing a generalised process and appropriate quality requirements for samples collected across the full mining value chain. The main goal of a quality programme is highlighted: to preserve, quantify and ensure sample representativity.

QM refers to reliable proactive detection of such "anomalous tendencies"; that is, the *trend* over time/grade of a given statistic. QM specifically also includes the process by which these trends are understood, communicated and rectified. Some businesses refer to this process as "continuous improvement" or as the "Plan–Do–Check–Act" cycle. In the mining industry, this proactive approach can have significant impact on financial outcomes through sequence optimisation, contract negotiation, and management of plant and processing infrastructure.

Examples of QM in the mining value chain

Below are presented examples of how QM can be implemented throughout the mining value chain, using a proactive approach as guided by JORC Table 1 (http://jorc.org/docs/JORC_code_2012.pdf#page=26) and how results are typically presented in QA/QC reports or audits.

Sampling ("sample collection")

JORC Table 1 provides guidance that drilling campaigns shall deploy measures to maximise sample recovery and representativity. A typical example for a reverse circulation (RC) drilling campaign would be to compare actual sample weights to a theoretical "ideal" drilling recovery, as a function of material density, rod length and diameter, and aperture size of the sample shoot (Figure 3).

Where duplicate samples are collected, it is expected that they will have similar, if not identical, sample weights. This is considered a satisfactory indication that the rig set-up, sampling devices and drilling/sample collection process are operating according to design, Figure 4.

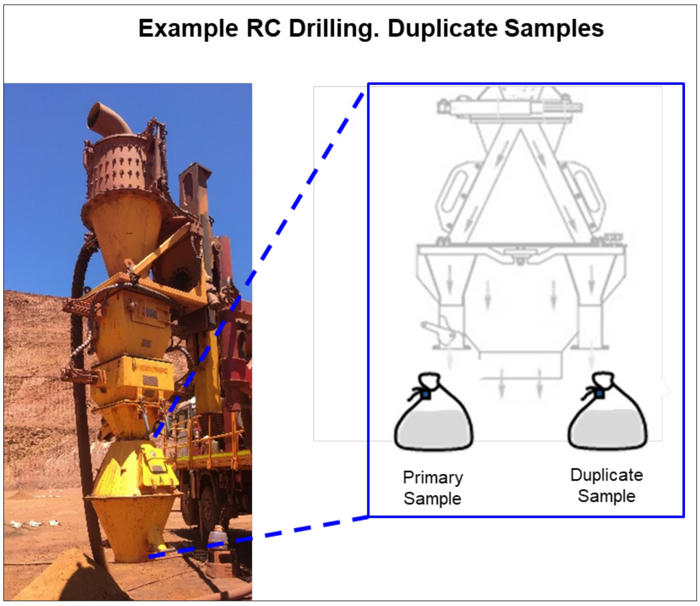


Figure 4. Duplicate field sample production directly at RC drilling site is considered a satisfactory sampling quality assurance if weight are closely similar.

Results are commonly presented as in Figure 5, in which a *scatter plot* shows the distribution of the results between duplicates. In this example, the scatter plot shows differences in weight outside expected thresholds, between 10 kg and 30 kg; and potentially a small bias towards to sample A being heavier than sample B.

However, there are several questions this graph *fails to answer*: why are A samples systematically larger than B samples? Is this the consequence of a particular drill rig? Or of a particular sampling device? When was the bias first introduced? Is this bias random, or sustained for a period of time? What was done to fix it?

Figure 6 presents an example of how QM practices can proactively improve sample collection by monitoring rig performance in a different way, while still comparing the weight of duplicate samples.

Figure 6 can be interpreted as follows: during the first two weeks of drilling in February, weight differences in rig 1 were not performing within accepted thresholds (Relative Difference ± 20 %). A conversation with the drill crew and drilling company supervisor is conducted in the field to explain to the driller the importance of drilling on geological models, to understand the sources of this poor performance, develop an action plan to improve the sampling practice and obtain a commitment to increase sample quality.

Through QM, corrective actions are taken by continuously monitoring results over time. This proactive approach can save thousands of dollars by "doing things right the first time" rather than reviewing QA/QC performance *en masse* once the drilling campaign is already finished, by which time it is too late, by far!

Sample preparation

Following the same criteria as for Sampling above, the JORC Table 1 benchmark requires evidence that "quality control procedures [are] adopted for all sub-sampling stages to maximise representivity of samples".

Usually, *blanks*, *duplicate samples* and *sizing tests* are used as a QA tool to monitor the performance of crushers and mills. Later, results are included on QA/QC reports where the performance of crushers and mills are summarised, for example as shown in Figure 7.

While these graphs and summary tables are typical in a great many mining practices today, this information does not allow the application of QM to monitor the information in real time and proactively improve the results. How can an

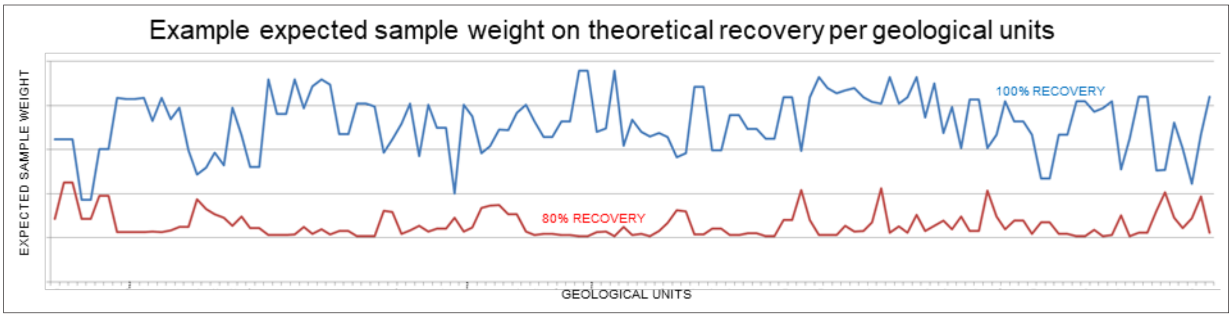


Figure 3. Comparing actual sample weights to a theoretical "ideal" drilling recovery.

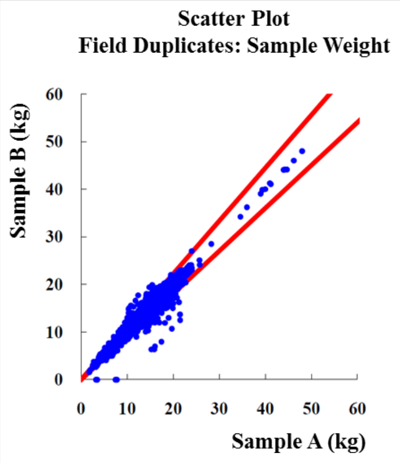


Figure 5. RC field duplicates performance: scatter plot comparison of duplicate sample weight.

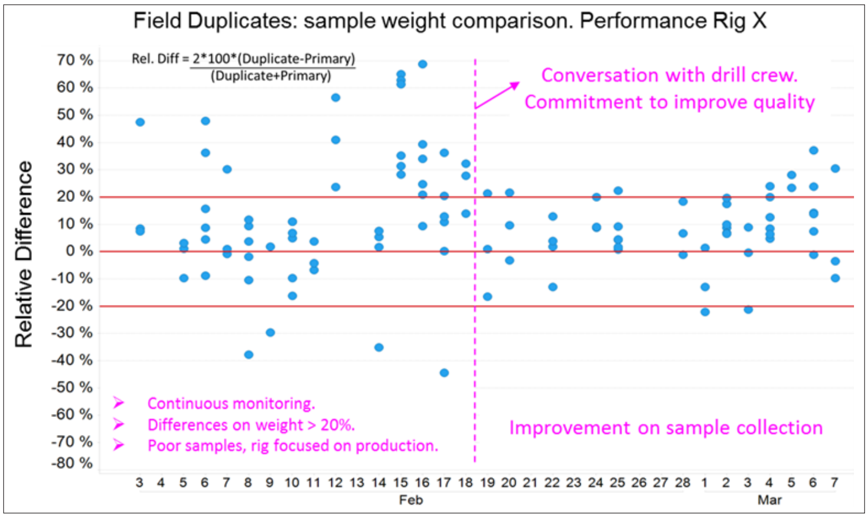


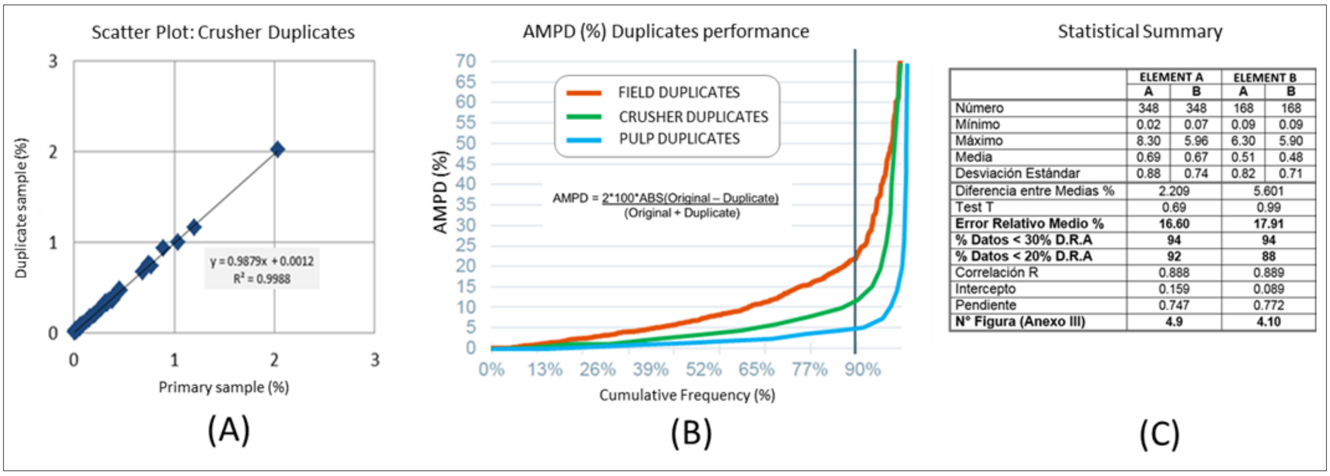
Figure 6. Example of monitoring sample weight on duplicate samples. Quality Assurance (QA): collect sample weight on duplicate samples. Quality Control (QC): sample weight within ±20% relative difference. Quality Management (QM): continuous monitoring of the information and actions were results are outside expected thresholds.

improved practice be designed and implemented? Again, time/grade-related trends are key!

Figure 8 shows an example where a trend analysis is performed both on a time (date) and on a grade basis: A) The Absolute Difference of Duplicate samples is plotted against the date the laboratory has reported the results. The graph does not show major issues over a specific period of time, but if the data is assessed on a grade basis as shown in B), a trend can be in fact be observed and interpreted as the grade of the primary sample being greater than the duplicate sample. The action here will be to talk to the drilling company (if these are field duplicates); or with the team performing the core cutting, or with the laboratory if the data are crusher or pulp duplicates—in order to find the *source* of this bias, and develop an action plan to fix and close the gap. This real-time assessment and management is the basis for the desired proactive approach. It needs to be highlighted, supplementing reactive activities such as reconciliation results or monthly/quarterly QA/QC reports (if done), where the opportunity for fixing issues in near-real time is lost.

Chemical determination

Certified Reference Materials (CRMs) are extensively used to monitor laboratory performance, and mining companies are obliged to arrange preparation of their own internal Working Reference Materials to perform QM. It is *not* recommended to rely on *internal* laboratory QA/QC processes only. Changes in the lab results or consistent biases across time are best detected by an *external* team accountable for QM, in order to highlight issues within the laboratory, to identify *sources* of deviations and their production consequences,



	ELEMENT A		ELEMENT B	
	A	B	A	B
Número	348	348	168	168
Mínimo	0.02	0.07	0.09	0.09
Máximo	8.30	5.96	6.30	5.90
Media	0.69	0.67	0.51	0.48
Desviación Estándar	0.88	0.74	0.82	0.71
Diferencia entre Medias %	2.209		5.601	
Test T	0.69		0.99	
Error Relativo Medio %	**16.60**		**17.91**	
% Datos < 30% D.R.A	**94**		**94**	
% Datos < 20% D.R.A	**92**		**88**	
Correlación R	0.888		0.889	
Intercepto	0.159		0.089	
Pendiente	0.747		0.772	
N° Figura (Anexo III)	**4.9**		**4.10**	

Figure 7. Examples of how duplicate samples performance are presented in QA/QC reports. (A) and (B) show different type of graphs to visualise and determine the correlation of the samples (A) and the % of data (B) on a certain % of difference, expressed as AMPD.

and to generate an action plan and apply lessons learned to avoid repetitive issues.

Often statistical analyses consider "average values", which sometimes lead to inaccurate conclusions that assume a process is well controlled "on average", or "fit for purpose". QM applies a different approach, assessing data in real time, thereby escaping the use of time-averages, and keeping an appropriate business focus with the aim to ensure consistent and defensible results, supporting sustainable business decisions.

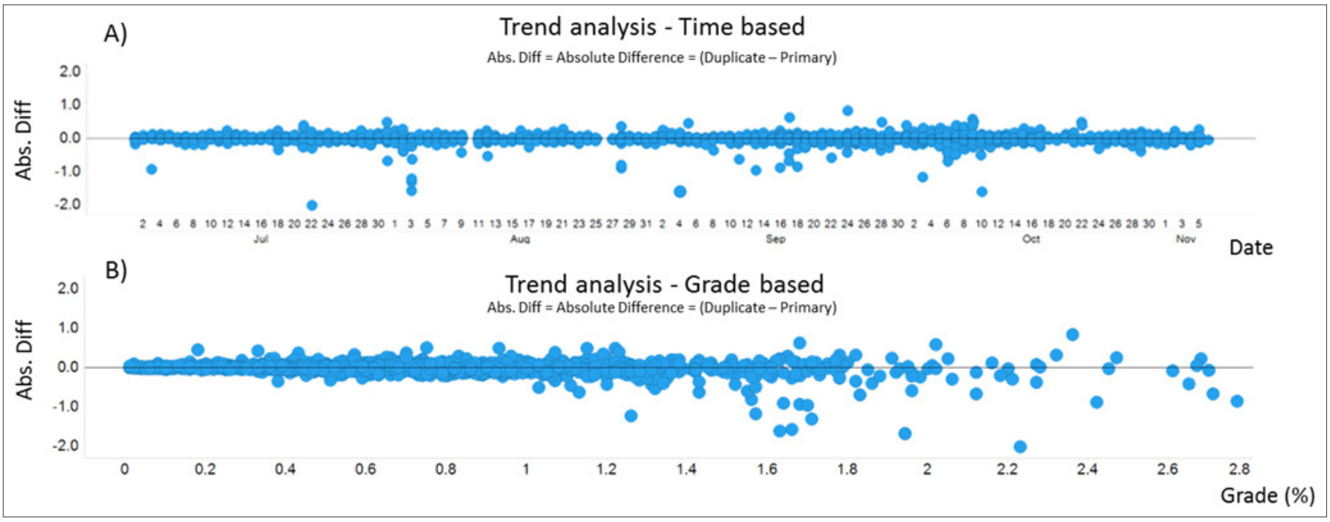


Figure 8. Examples of trend analysis performed on a time and grade basis for duplicate samples (applicable for field, crusher and pulp duplicates). These graphs highlight the value of performing QM both on a date and grade basis: the analysis by time (date) does not reveal any major issue in terms of bias and the results look consistent. However, trend analysis performed on a grade basis highlights a bias at high grades that needs to be reviewed, understood and fixed.

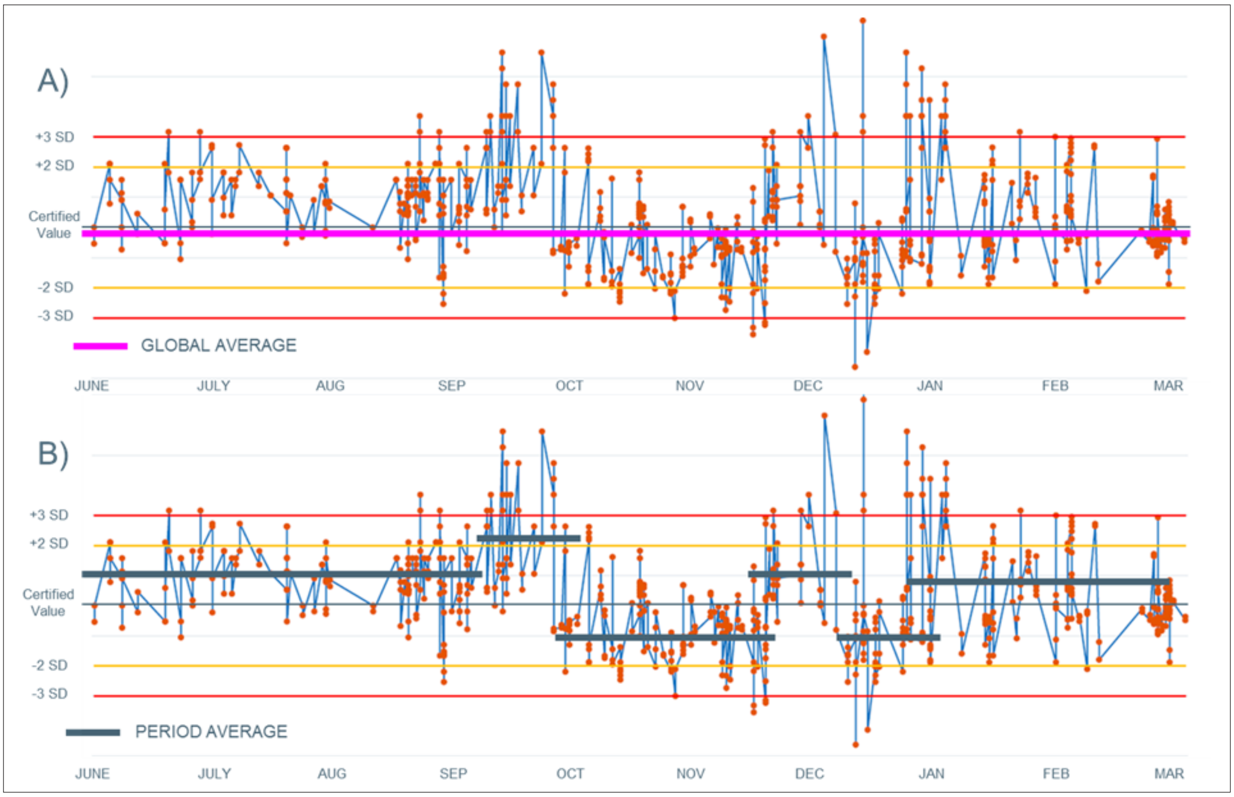


Figure 9. CRM performance showing results performing mostly *within* three expected standard deviations. A) Global average is very close to the certified value, which can be interpreted as the results are considered valid. B) Period average has been included, showing the significant time-variability of the laboratory performance during individual months.

Figure 9 demonstrates the differences between an approach reliant on averages vs QM applied to CRM results (QA = CRMs, QC = ±3SD and QM = trend analysis). Figure 9A shows 10-months' performance of a CRM. Because results have been performing mostly within three standard deviations, the business might infer the process is well controlled and would feel confident, given the global average is close to the certified value.

However, Figure 9B shows the internal variability which the laboratory (period average) is observing over time. This lack of consistency gives rise to operational instability, exposing the business to risks of under- or over-performing at production, processing and compliance to plan results, or leads to variable products.

These are examples of cases where QM becomes important by monitoring information in real time and detecting changes in the performance of the laboratory proactively, thereby ensuring consistency and sustainability of business results.

Conclusions

This column highlighted that a quality programme is not just a statistical exercise, where global averages or standard deviations assure sustainable and consistent QA/QC results. The examples provided demonstrate the value of QM to *complement* routine QA/QC processes and statistical analysis, enabling a QM proactive approach in which data monitoring will ensure consistent results across time or, over a range of grades, will reduce resource and operational risks, and allow business decisions based on representative and quantified-quality information across the entire value chain.

Indirectly this paper also highlights the value and necessity of having a central (external) QM team which is accountable for governance and for performing appropriate quality-related activities (QA/QC and QM) *across* both exploration and production.

Finally, QM is currently *in vogue* and companies have been pushing to be part of "a new era" of new technological applications (sensors) and data analysis (machine learning, conditional simulations etc.), which is trying to provide businesses with real-time data to be used for business decisions in real time etc. This column highlights that both new technology and advanced statistical techniques *need* to be based on appropriately defined "good quality data", not just a lot of data. Appropriately good data also needs to be incorporated into simulations and advanced statistical tools. QM becomes a critical success factor to ensure that performance of future technologies are robust—otherwise the old adage still rules: Garbage In–Garbage Out (GIGO).

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Geologist, Master of Business Administration (MBA), and Geo-Mining-Metallurgical Diploma, with >20 years of international experience developed in the mining industry and multi commodities. Council member of the International Pierre Gy Sampling Association (IPGSA). 16 years working in BHP, currently as Global Principal Geoscientist QAQC, at the Technical Centre of Excellence, providing support on Sampling & QAQC to all the assets and commodities of BHP.

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APPLICATIONS

Analysis of hand sanitiser products using 1064`nm handheld Raman

Rigaku Analytical Devices has published a new application report detailing the analysis of hand sanitisers. This describes the analysis of hand sanitiser products by Raman spectroscopy and highlights the performance of the Rigaku portfolio of handheld Raman analysers. The use of hand sanitisers is becoming part of the everyday norm, and global demand has grown significantly. As hand sanitisers in liquid and gel formulations are being produced by manufacturing companies around the world, there is a global focus on hand sanitiser manufacturing and quality control to ensure that they do not contain hazardous chemicals or fail to provide adequate protection. In response to increased consumer demand, regulatory agencies have also put processes in place to monitor import/export activity, as well as to directly test suspicious shipments.

The two main active ingredients in most commercially available alcohol-based hand sanitisers are ethyl alcohol (ethanol) and isopropyl alcohol (isopropanol). These chemicals, as well as many potentially dangerous contaminants commonly found in handheld sanitiser formulations, are reactive to Raman spectroscopy. 1064 nm Raman analysers are also favourable because of their ability to analyse finished products through coloured packaging, such as blue and green-tinted plastic or glass, as well as identify the chemicals used during manufacturing.

Rigaku Europe

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Chemical reaction feedstock troubleshooting with benchtop NMR

Benchtop NMR has many advantages over similar analytical techniques due to its high degree of chemical specificity, especially when combining information from multiple chemical nuclei. Minimal or no sample preparation and quick data generation allows the deployment of benchtop NMR in QA/QC environments without the need for operation by R&D scientists. This saves significant time and money. One example is in the quality control of reaction feedstocks which are the raw chemical materials required to supply large-scale chemical manufacturing processes.

Oxford Instruments

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Identification of microplastics using Raman spectroscopy

Microplastics are found everywhere in the environment including oceans, fish, salt, air, rivers, bottled water and tap water. They accumulate in water and are eaten by animals such a fish and shellfish. These microplastics are then subsequently found in food and water for human consumption. There is a lot of debate and research around how dangerous microplastics are to the human body and, so far, the results are inconclusive.

Raman spectroscopy is ideal for distinguishing polymers, contaminants and dyes. Its fingerprint type analysis offers great potential as a tool in identifying microplastics in marine environments. Commonly employed techniques for studying microplastics are often limited to particle sizes above 300 µm. However, only particles smaller than 150 µm can be absorbed into the human gut and, therefore, this size range could be of vital importance. The high spatial resolution offered by confocal Raman spectroscopy means even the smallest of microplastics can be interrogated.

This application note investigates three polymers, polyethylene (PE), polytetrafluoroethylene (PTFE) and nylon-6. PE is one of the most manufactured polymers, with tens of millions of tonnes made globally each year, much of this being used in packaging, and is one of the top three most commonly found plastics in global aquatic systems. PTFE is a fluoropolymer used frequently for its non-stick properties, for example in frying pans. PTFE shares a very similar structure to PE, however, their synthesis and uses differ significantly. There have been several cases recently where perfluorooctanoic acid (one of the synthesis materials for PTFE) has been found in drinking water in the USA and Australia, this acid is a carcinogen. Nylon-6 is a polyamide which frequently finds use in the automotive industry and in fishing materials. These three polymers were chosen for their abundance in the Earth's oceans.

Edinburgh Instruments

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Multi-nuclear PFG spectroscopy on a benchtop NMR spectrometer

Molecular diffusion is the mechanism that defines molecular mobility in solutions. The study of diffusion processes is of interest in widespread fields in science where transport of mass needs to be determined. NMR is the method of choice to quickly determine self-diffusion coefficients of chemical species in solution. A commonly used NMR technique requires the combination of pulsed field gradients with a stimulated echo sequence (PGSTE). The spectroscopically resolved version of this sequence makes it possible to measure the diffusion coefficient of different molecules in a mixture by measuring the diffusion attenuation of the signal of each particular chemical group of each molecular structure.

Magritek

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Real time analysis of multiple compounds in human breath

The use of VOCs as a real-time marker in human breath for physiological events such as lactate threshold, and oxidative stress is a challenge for conventional "off-line" gas analysis equipment, such as GC/MS. The analysis necessitates very fast response, coupled with a wide dynamic range. The HPR-20 TMS Transient mass spectrometer is ideal for this application due to the fast response, wide dynamic range and high sensitivity offered by the PIC detector.

Hiden Analytical

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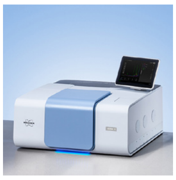

APPLICATIONS: Research ▪ Development ▪ Analytical science

KEY FEATURES: Integrated touch panel ▪ MultiTect detector technology ▪ Transit measurement channel ▪ Spectral range from 15 cm^{-1} to 28,000 cm^{-1} ▪ Unique Bruker FM technology

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APPLICATIONS: Pharma ▪ Materials identification ▪ Incoming goods control

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APPLICATIONS: Spectrophotometer for scattering samples ▪ Effective scattering coefficient and absorption coefficient

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KEY FEATURES: 200–1100 nm ▪ Size of a deck of cards ▪ Easy to integrate ▪ Suitable for harsh environments ▪ USB powered ▪ Temperature & wavelength stability ▪ 2048 or 4096 pixel detector

PRODUCT: New HySpex SWIR-640—SWIR Hyperspectral Imaging Camera

APPLICATIONS: Laboratory ▪ Field ▪ Airborne ▪ Geology ▪ Vegetation ▪ Mining ▪ Food quality ▪ Military

KEY FEATURES: Universal ▪ Sharper optics ▪ Greater spectral fidelity per pixel at an affordable price ▪ 640 special pixels ▪ 360 spectral bands

PRODUCT FOCUS

PRODUCT: **Imec snapshot SWIR Hyperspectral Imaging Camera**
APPLICATIONS: Optical sorting in machine vision ▪ Security & surveillance ▪ Chemical analysis of materials ▪ Food safety ▪ Medical ▪ Pharmaceutical ▪ Semiconductor & PV ▪ Recycling ▪ Minerology & mining ▪ Vegetation
KEY FEATURES: Video-rate acquisition of hyperspectral data cubes with no motion artifacts, perfectly suited for acquisition of moving objects or scenes ▪ Easy set-up of the complete system ▪ Flexible configuration

Quantum Design
Tel: 01372 378822
info@qd-uki.co.uk
www.qd-uki.co.uk

PRODUCT: **ILT 960-UV Portable Compact UV Spectrometer**
APPLICATIONS: Validating your UVC disinfection system ▪ Use UVC light to decontaminate air, water, surfaces and personal protective equipment (PPE) or other devices
KEY FEATURES: Measures UV light levels as small as 0.4 uW/cm^2/nm

PRODUCT: **Raptor Ninox 640 SU SWIR Cameras**
APPLICATIONS: Astronomy ▪ Beam profiling ▪ Hyperspectral imaging ▪ Semiconductor inspection ▪ Solar cell inspection ▪ Thermography ▪ Microscopy ▪ Art inspection
KEY FEATURES: Vacuum cooled to –80°C enables ultra-long exposure times ▪ Ultra-low dark current and read-noise resulting in the highest sensitivity SWIR camera on the market

PRODUCT: **Moxtek Infrared Polarisers**
APPLICATIONS: UV curing and projection display applications
KEY FEATURES: Configurable for high transmission or high contrast performance ▪ Custom sizing available ▪ Wavelength independent performance (broadband models) ▪ Wide acceptance angle (± 0°)

Specac Ltd
Tel: 01689 873134
hazel.hall@specac.co.uk
www.specac.com

PRODUCT: **Quest High Throughput Accessory ATR**
APPLICATIONS: Pharmaceutical ▪ Biodiesels ▪ Polymers and chemistry ▪ Paint ▪ Legal and illegal narcotics
KEY FEATURES: Innovative optical design ▪ All reflective gold-coated optics ▪ Synopti-focal array technology ▪ Precision-moulded aspheric mirrors

S.T.Japan-Europe GmbH
Tel: +49 (0)2234 956372
contact@stjapan.de
www.stjapan.de

PRODUCT: **Spectra Databases**
APPLICATIONS: Material & substance identification ▪ Multilayer analysis ▪ Failure analysis ▪ Microplastics analysis ▪ Composition investigation
KEY FEATURES: ATR-FTIR, Raman, NIR spectra ▪ Broad range of substances ▪ Compatible with all instruments & search software ▪ Fixed Costs—pay only once ▪ Permanent license

PRODUCT: **Sampling Knives**
APPLICATIONS: Multilayer analysis ▪ Surface analysis ▪ Failure analysis
KEY FEATURES: Precise cutting with diamonds ▪ Thinnest surface cuts ▪ Cleanest cross sections ▪ Easy removal of surface contaminations

PRODUCT: **Diamond Compression Cell**
APPLICATIONS: Transmission analysis of micro solid samples ▪ Excellent for analysing hard materials such as minerals, rubbers, plastics, polymers & pharmaceuticals
KEY FEATURES: Large clear sperture ▪ Two synthetic diamonds Type IIa ▪ Excellent transmission from UV through Far-IR spectral region ▪ Universal use with FTIR spectrometers & microscopes ▪ Easy to assemble and clean

Starna Scientific Ltd
Tel: +442085001264
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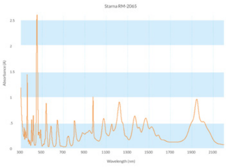
PRODUCT: **FTIR, ATR & Mid-IR Certified Reference Materials (Polystyrene films)**
APPLICATIONS: Wavenumber/resolution calibration ▪ European Pharmacopoeia & USP validation ▪ Calibration ▪ FTIR & ATR ▪ Mid-IR
KEY FEATURES: ISO/IEC 17025 accredited (UKAS) ▪ NIST traceable ▪ 3 year validity

PRODUCT: **NIR, Mid-IR Certified Reference Materials (Metal-on-Quartz & Neutral Density Filters)**
APPLICATIONS: Photometric accuracy ▪ European Pharmacopoeia & USP validation ▪ NIST traceable ▪ NIR ▪ Mid-IR
KEY FEATURES: ISO/IEC 17025 accredited (UKAS) ▪ NIST traceable ▪ 2 year validity

PRODUCT: **Wide-Range Wavelength Reference (335 nm to 1945 nm)**
APPLICATIONS: Wavelength accuracy ▪ European Pharmacopoeia & USP validation ▪ NIST Traceable ▪ NIR
KEY FEATURES: ISO/IEC 17025 accredited (UKAS) ▪ NIST traceable ▪ 2 year validity



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PRODUCT: **trinamiX Mobile NIR Spectroscopy Solutions**
APPLICATIONS: Plastic sorting ▪ Animal nutrition ▪ Skin and hair care ▪ Materials and substances ▪ Food
KEY FEATURES: Portable (fits into your hand) ▪ Fast results ▪ Cloud-connected app ▪ Ready-to-use ▪ Wavelength range: 1400 nm to 2500 nm

Viavi Solutions Inc.
Tel: +1 800 254 3684
ospcustomerservice@viavisolutions.com
micronir.com

PRODUCT: **MicroNIR OnSite-W Handheld NIR Spectrometer**
APPLICATIONS: Raw material ID ▪ Food, feed and agriculture ▪ Illicit materials ID ▪ Counterfeit detection
KEY FEATURES: Wireless handheld ▪ Lightweight and ergonomic ▪ One-button operation ▪ Long battery life ▪ Robust IP65/67

PRODUCT: **MicroNIR PAT-W Wireless Process NIR Spectrometer**
APPLICATIONS: Pharmaceutical manufacturing ▪ Tumble blending ▪ Tableting & compaction ▪ Wireless monitoring
KEY FEATURES: Wireless WiFi connected ▪ Lightweight and robust ▪ Multiple triggering modes ▪ IP65/67 rated ▪ ATEX/IECEx-rated option

PRODUCT: **MicroNIR PAT-L Immersion NIR Spectrometer**
APPLICATIONS: Polymer processing ▪ Petrochemicals ▪ Oil & gas ▪ Biopharma
KEY FEATURES: Fully integrated spectrometer & immersion probe ▪ Multiple configurations for diverse applications ▪ USB power & data ▪ ATEX/IECEx-rated option

NEW PRODUCTS

ATOMIC

New SPECTROGREEN TI ICP-OES analyser

SPECTRO Analytical Instruments has introduced the latest version of its SPECTROGREEN inductively coupled plasma optical emission spectrometry (ICP-OES) analyser, the SPECTROGREEN TI, which uses SPECTRO's twin interface (TI). This automatically combines both axial and radial plasma views, optimising sensitivity, linearity and dynamic range while avoiding matrix effects like those from easily ionisable elements. This enables the SPECTROGREEN TI to provide high sensitivity for trace elements, as well as freedom from matrix interferences plus good accuracy for challenging environmental matrices.
SPECTRO Analytical Instruments

- https://link.spectroscopyeurope.com/32-111

New ICP-MS system with smart tools

Agilent Technologies have announced a new ICP-MS instrument, the Agilent 7850 ICP-MS system, that provides new smart tools that bring advanced capabilities to the routine ICP-MS laboratory. If a lab fails to recognise or address common time traps, they may not just lose time and revenue. Unnecessary method setup steps, instrument checks, manual data reviews and the need for sample reanalysis also place more pressure on lab staff. This workload can impact sample turnaround time and the quality of the results. The 7850 uses a configuration that is optimised to handle the range of sample types measured in typical ICP-MS applications while ensuring data is free from common sources of error. Smart tools help customers through the initial setup of the instrument and required methods, and guides users through the typical ICP-MS workflow that is used to measure sample batches. Smart functions also assist with data review, eliminating the need for an ICP-MS expert to perform the important step of verifying data quality.
Agilent Technologies

- https://link.spectroscopyeurope.com/32-113

New multicollector ICP-MS system

The Thermo Scientific Neoma Multicollector inductively coupled plasma mass spectrometry (MC-ICP-MS) system has increased automation and a new variable detector array with 11 Faraday cup detectors. All Faraday cups are brought into precise alignment with ion beams of different dispersions, which enables coverage from Li to U, in low or high resolution and without compromising the native dispersion of the mass analyser.
Thermo Fisher Scientific

- https://link.spectroscopyeurope.com/32-109

IMAGING

Raptor Photonics Ninox 640 SU camera

Quantum Design UK and Ireland have announced that Raptor Photonics has launched the Ninox 640 SU, a vacuum-cooled InGaAs-based camera with 640 × 512 sensor with a 15 × 15 µm pixel pitch for high spatial resolution. The Ninox 640SU is vacuum cooled to –80 °C for long exposures of up to 5 min. It is suitable for staring applications in SWIR wavelengths (900–1700 nm) including NIR-II *in vivo* imaging, fluorescence imaging and astronomy.

Quantum Design UK and Ireland

- https://link.spectroscopyeurope.com/32-116

New series of hyperspectral cameras

The collaboration between imec and XIMEA has resulted in a series of new hyperspectral cameras (xiSpec2). For five years, XIMEA has commercialised imec's hyperspectral technology in its xiSpec cameras. These have the capability of real-time video rate spectral data acquisition, enabling new applications where traditional push-broom is too challenging. The xiSpec2 camera is targeted at the medical, agriculture and machine vision markets, and imec is taking an active role in the collaboration. XIMEA and imec optimised the camera design to improve the spectral quality of the acquired data and enable customers to tailor image quality and spectral range to their application. Also, new software enables applications in more challenging, non-standardised industrial settings. The xiSpec2 series consists of three standard cameras as well as the custom solutions. Customers can obtain a starter kit with the necessary peripherals (lenses, cables etc.) to ensure a smooth startup as well as after-sales support that includes a warranty on the spectral image quality. Finally, xiSpec2 camera customers have access to imec's manuals, sample data and technical support.

imec

- https://link.spectroscopyeurope.com/32-114

MASS SPEC

Pfeiffer Vacuum introduces new turbopumps

Pfeiffer Vacuum's HiPace 350 and 450 turbopumps are dedicated for applications like mass spectrometry, electron microscopy, metrology tools, particle accelerators and plasma physics, as well as coating, R&D and industrial applications. HiPace 350 and 450 have low weight and a small footprint. They are based on a hybrid bearing, a combination of ceramic ball bearings on the forevacuum side and permanently magnetic radial bearings on the high vacuum side. The rotor design of the turbopumps results in a high pumping speed for light gases. High backing pump compatibility and high gas throughput as well as excellent compression for light gases are made possible by the rotor design.

The integrated HiPace drive electronics offer a variety of communication interfaces, including ProfiNet and EtherCat without any increase in physical size. Remote and sensor functionalities allow the analysis of pump data, such as temperatures. The pumps are certified to Semi S2, UL, CSA and Nema 12. Bearing maintenance on-site is possible. Bearing exchange can be done on the customer's site and the pumps can run for up to four years without service.

Pfeiffer Vacuum

- https://link.spectroscopyeurope.com/32-115

NIR

Portable NIR for raw material and feed analyses

Evonik has launched AMINONIR® Portable, a mobile NIR service for amino acid calibrations using Viavi's MicroNIR handheld spectrometer. AMINONIR® Portable enables the determination of energy, nutrients in feed raw materials and feed, as well as amino acids in feed raw materials, on-site and independent of a laboratory. The hand-held device connects with the user's tablet or cell phone and only requires mobile signal reception and a handful of feed or raw material without further sample preparation to determine their quality at almost any location within minutes. AMINONIR® Portable can be used to analyse over 40 different feed raw materials and feed mixtures for broilers, laying hens, pigs and fish. It significantly extends the application of NIR spectroscopy, which Evonik has been offering as AMINONIR® services for 25 years.

Evonik

- https://link.spectroscopyeurope.com/32-110

UV/VIS

Portable compact UV spectrometer

Quantum Design UK and Ireland have introduced International Light Technologies' ILT 960-UV to the UK and Ireland market. The ILT 960-UV is ILT's new portable, compact UV spectrometer with increased broadband sensitivity. The ILT 960-UV can measure UV light levels as small as 0.4 uW cm^{-2} nm^{-1}. The ILT 960-UV-RAA4 includes the spectrometer, 1-m fibre-optic light guide, RAA4 right angle cosine correcting input optic, calibration with certificate and carrying case. UV germicidal irradiation systems depend on the proper intensity of light reaching a surface to ensure proper disinfection. The new ILT 960-UV is combined with ILT's SpectrILight III software, which includes a baseline overlay comparison, irradiance select and peak find.

Quantum Design UK and Ireland

- https://link.spectroscopyeurope.com/32-112

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X-RAY SPECTROMETRY

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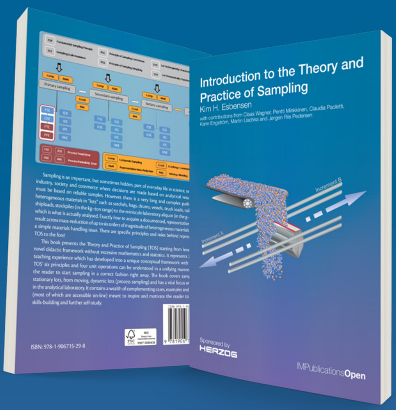
Introduction to the Theory and Practice of Sampling

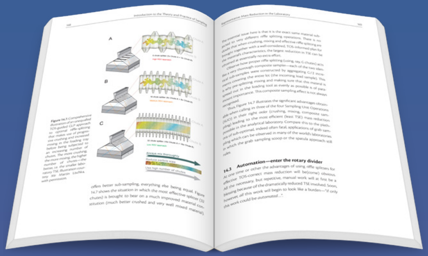
Kim H. Esbensen

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.

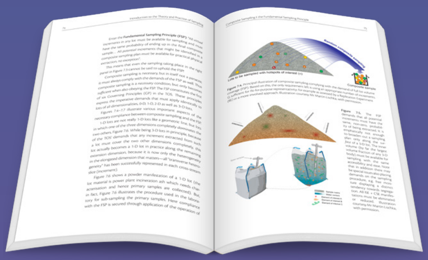




"I recommend this book to all newcomers to TOS"

"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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