ISSUE 1/2016

X'PRESS

PANalytical
get insight

Welcome to the latest issue of **X'Press**

Pieter de Groot
Corporate marketing director

The theme in this first edition of the new year is trust. Trust, in the meaning of 'relying on' or 'having faith in' is from all times and is in my opinion the base of all relationships in personal and business life.
Can a company be trusted? Judging from the many long-term customers we have, I dare to say that many of our customers do trust PANalytical – but why is that? Like Gjalt Kuiperes points out in our interview, we do as we promise, make sure that our systems are delivered strictly in time and with the correct specifications and if not we take responsibility for it. Additionally our customers seem to appreciate the high ethical standards we are applying to all our actions; an important aspect in the present global business world where mutual trust is highly valued.

Our relation with the customer does not end with the delivery of a system, it is only the start of it! Subsequently our engineers make sure that the system is installed correctly and is functioning without problems; they instruct the users and assist with setting up the desired applications.

And there is more – in case of any problems, either with the system or the application, our people will be able to help any time; help which is now facilitated by our new Remote Assistance Suite. This way you can always be sure that your analytical results can be trusted.

PANalytical's systems usually serve yet another aspect of 'trust': they enable the user to trust the quality of his products. Our stories about banah UK Ltd., SoilCares and the Indian Hetero Drugs company show how these customers use our equipment for quality control. Does the newly developed cement contain the desired components, what is the exact composition of the analyzed soil and do the produced drugs only contain the specified compounds in their effective form – these are only some of the questions which can be answered by employing X-ray diffraction or X-ray fluorescence.

Another area where trust is the base of the entire process is research. From defining your research problem to measuring and publishing the results, trust is the base value. The researchers in Prof. Goodwin's lab in Oxford, UK, are using PANalytical's newest detector, the GaliPIX^{3D}, to explore the disordered state of materials by pair distribution function analysis. This technique will soon enable analyses which have not been possible in the past when X-ray diffraction results could only be trusted when applied to crystalline materials.
It fascinates me how even a traditional technique as X-ray materials analysis can be employed for new applications we had not heard of a few decades ago.

With kind regards,
Pieter de Groot

LATEST NEWS

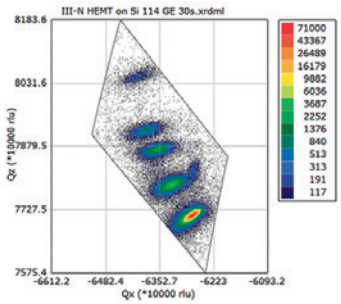
Ultimate speed of reciprocal space map measurements

Until recently reciprocal space map (RSM) measurements were considered too time-consuming for quick structural analysis of layered materials.

Now, ultra-fast reciprocal space mapping (URSM) is available in the new Data Collector (version 5.3). A URSM can be collected with any of PANalytical's available 2D detectors, for instance PIXcel^{3D}, in acquisition times comparable to rocking curves without compromising data quality.

RSMs can reveal additional valuable information beyond that provided by single line scans such as commonly used for high-resolution rocking curves.

For more information visit the knowledge center on our website and watch how a URSM is collected in less than 30 seconds.
www.panalytical.com/Technology-background/rsm.htm



Ultra-fast reciprocal space map collected in 28 seconds

In this issue

PANalytical makes its mark in **geopolymer cement** with banah UK Limited

Cement is economic, efficient, versatile and durable, and widely acknowledged as THE building material. However, cement manufacture causes environmental impacts at many stages of the process. Quarrying can damage the countryside and emits airborne pollution such as dust, gases, noise and vibration. The traditional cement industry is one of the largest producers of CO_2 globally. This is partly due to the burning of calcium carbonate, producing lime and carbon dioxide. The other part is the high use of energy which is a potential CO_2 contribution if the energy production has involved emission of CO_2. Reducing CO_2 emission is one of the biggest challenges for today's construction industry.

banah UK Limited, based near Coleraine in Northern Ireland, has taken up this challenge and following an intensive five-year R&D program, has developed a material that is considered to be an improvement over traditional cement both in its intrinsic properties and it's lower carbon footprint. It is based on a so-called geopolymer and it mimics natural rock formations, such as basalt.

Known also as an alkali activated cement, it consists of two components, a powder banahCEM(A) and a liquid activator banahCEM(B). The resulting geopolymer cement is heat-resistant; it does not spall and tolerates much greater temperatures than ordinary Portland cement. Additionally it has increased acid and sulfate resistance and a rapid strength gain during setting.

The long-term durability of banahCEM is a direct consequence of its replication of natural rock formations.

Furthermore, banahCEM is environmentally friendly. To produce it, 80% of carbon emissions are eliminated when compared to ordinary Portland cement. The excavation of raw materials for banahCEM has at least 60 % less impact on the environment and it uses waste materials or by-products from existing industries.

banah UK purchased a PANalytical X'Pert^3 Powder diffractometer at the beginning of 2015. The measurements reveal information about the crystallographic structure, composition and properties of the material. The system is an essential part of the company's quality control system and also an important tool in the research and development of new products.

It has helped scientists at banah UK Limited to make informed decisions in their pilot plant, and subsequently, for their main plant, which is currently entering the commissioning phase and should be in production by mid-April.

banah UK Limited, with the help of PANalytical, are cementing the future in building materials.

"The expert training and advice from PANalytical has proven invaluable for us as we start out in the complicated field of clay mineral analysis."

- Andrew McIntosh,
Director of R&D, banah UK Ltd

Andrew McIntosh (Director R & D),
Dr. Susan Lawther (Geologist),
Terry Soteriou (PANalytical)

Cement

Cement has been around since the Roman times, when they used a mixture of volcanic ash (pozzolana) and burnt lime to make 'opus caementicium' or Roman concrete.

At present the most common type of cement is ordinary Portland cement, made by heating limestone (calcium carbonate, $CaCO_3$) with other materials such as clay up to 1450 °C to form calcium alumosilicates and other cementitious compounds. The resulting 'clinker' is then ground with a small amount of gypsum into 'ordinary Portland cement'.

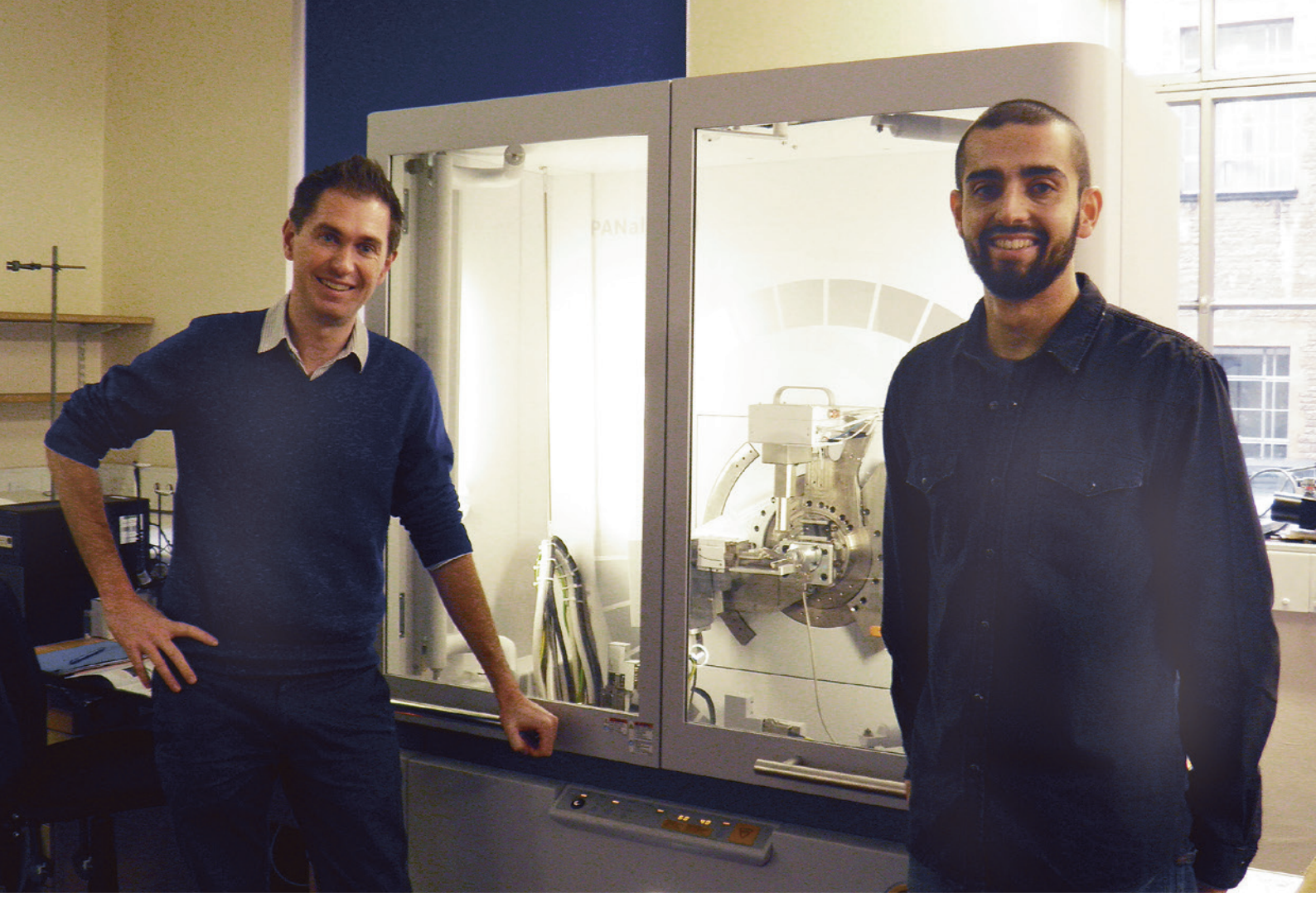
Other cement types contain additions of blast furnace slag, fly ash or limestone. Volcanic ash is still used, when cheaply available. Geopolymer cement relies on minimally processed natural materials or industrial byproducts to significantly reduce its carbon footprint.

banah UK Ltd
Cement Reimagined

banah UK Ltd was established in 2008 with one clear aim: to find better ways of building. In 2013 the company received additional investments of over £ 5 million which is being used to create a new state-of-the-art R&D and manufacturing plant near Coleraine, Co Londonderry, Northern Ireland.

banah UK Ltd. currently employs 13 staff, with the potential to create up to 10 new jobs in the next two years.

banah UK Limited is committed to continue research & development in the field of geopolymers and sustainable building materials and to expanding, developing and improving its products.



Andrew Goodwin (left) with student Harry Geddes

PDF analysis: A twenty-first century revolution?

We celebrated the Bragg centenary in 2014 and this year we celebrate the Golden Jubilee of Rietveld. These anniversaries remind us that the twentieth century marked some real advances towards the understanding of the ordered crystalline phase in materials. However, there are still many unanswered questions about the regions in solids that are not ordered. Professor Andrew Goodwin and his group in the Inorganic Chemistry Laboratory of Oxford University, UK, make it their purpose to understand and exploit the ways in which atomic disorder gives rise to a variety of interesting physical properties in crystalline and amorphous solids of both commercial and scientific importance.

Disorder occurs in all materials. For example disorder occurs around defects in crystals and at the grain boundaries of polycrystalline materials. At any one moment in time a single crystal will have some atoms displaced from their average lattice position: this kind of disorder is vital for phase transformations to occur. Some materials simply don't form crystals and exist as glasses or amorphous solids.

In all of these cases, whilst the material or region under study may not have a perfect crystalline lattice, certain atom-to-atom distances are repeatedly maintained. These atom-atom correlations can be studied and provide useful information about materials and their structures.

One of the methods that Andrew Goodwin's group uses to investigate disorder is pair distribution function (PDF) analysis [1]. Andrew was PANalytical's first customer to receive a GaliPIX^{3D} detector for laboratory X-ray PDF measurements on an Empyrean difffractometer. Already the group has published papers using X-ray PDF data measured on this diffractometer [2].

Andrew is also chair of the user working group helping to develop a dedicated X-ray PDF beam line (XPDF) at the Diamond synchrotron facility, UK. He is clearly excited about the new synchrotron facility, which will be the first dedicated X-ray PDF beam line in Europe.

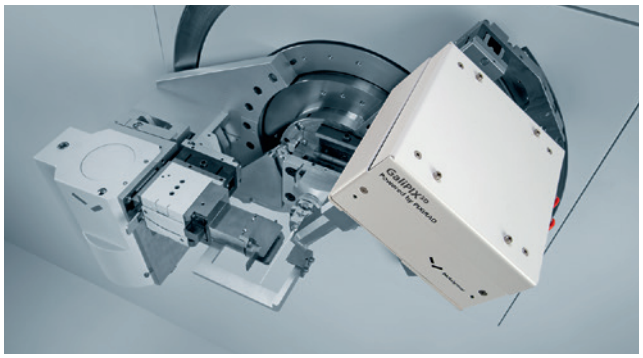
Andrew says it is a win-win situation to have access to a lab diffractometer in addition to beam time at a synchrotron facility: "Because we have a dedicated X-ray PDF instrument in the lab, we will use our synchrotron beam time more wisely. With an in-house instrument, users can go to the synchrotron better informed about their samples and with a clearer vision of what they want to achieve".

Prof. Goodwin's research group covers a large range of projects some of which include PDF studies. For example, student Harry Geddes is using X-ray PDF analysis to look at amorphous pharmaceuticals. In the absence of a crystalline fingerprint from Bragg peaks, the PDF method may, in the future, provide the basis for a standardised approach to the identification and quality control of some of the newest drugs in which we will place our trust.

PDF analysis

PDF analysis is becoming adopted for research in an ever increasing number of scientific areas where an understanding of disorder is important, for example:

- Phase transformations
- The absorption and desorption of gases
- The transport of ions in the anodes of batteries
- The electro-optical and magnetic properties of many advanced materials
- The trapping of methane and heavy metals in clays
- The discovery and characterization of drugs based on amorphous materials
- The biomineralization of amorphous species in the formation of bone and tooth enamel



GaliPIX^{3D} setup for a PDF measurement

References:

[1] Learn more about this subject from our application note 'Pair distribution function analysis' in the knowledge center on our website (www.panalytical.com/knowledgecenter)

[2] D. Umeyama, N. P. Funnell, M. J. Cliffe, J. A. Hill, A. L. Goodwin, Y. Hijikata, T. Itakura, T. Okubo, S. Horike and S. Kitagawa, Chemical Communications 51, 12728-12731 (2015); N. P. Funnell, Q. Wang, L. Connor, M. G. Tucker, D. O'Hare and A. L. Goodwin, Nanoscale 6, 8032-8036 (2014); M. J. Cliffe, W. Wan, X. Zou, P. A. Chater, A. K. Kleppe, M. G. Tucker, H. Wilhelm, N. P. Funnell, F.-X. Coudert and A. L. Goodwin, Nature Communications 5, 4176-(2014).

The **Inorganic Chemistry Laboratory in Oxford University** (UK) is the biggest school of inorganic chemistry in the UK and one of the biggest in the world. Whilst Prof. Goodwin and his group of about 20 researchers work with state-of-the-art equipment on the latest scientific challenges, their lab is found in a department with a long history of scientific enquiry.

It was home to 6 Nobel Laureates including Dorothy Crowfoot Hodgkin, who was awarded the Nobel Prize in 1964: 'for her determinations by X-ray techniques of the structures of important biochemical substances'. It is an inspiring setting in which to explore the frontiers of chemistry in the twenty-first century.

The front of the Inorganic Chemistry Laboratory, with the central blue hexagonal plaque celebrating Dorothy Crowfoot Hodgkin

Trusted soil quality from SoilCares

One of mankind's problems is the continuous growth of the world population, which is expected to hit 9 billion people in 2050. In order to fill the stomachs of that growing population a 70% increase in food production will be required. SoilCares firmly believes that a healthy local/regional food production will make food available worldwide. The company aims at enabling farmers all over the world to improve their yields by providing them with easy-to-use soil testing solutions leading to fertilizer and crop recommendations.

Lab-in-a-box is one of these testing solutions: a very compact laboratory based on sensor technology to perform soil tests. This laboratory can be installed in the boot of a car or on a farm.
The Lab-in-a-box uses two different techniques to analyze macro- and micro-nutrients in the soil: a mid-infrared (MIR) sensor and X-ray fluorescence (XRF), provided by PANalytical's Epsilon 1 benchtop spectrometer.

With this Lab-in-a-box soil tests are very easy to perform; people without any laboratory experience can analyze soil samples after a short training session. The results of this Lab-in-a-box are as accurate as those of traditional wet-chemical soil analysis.

The test results of the Lab-in-a-box are analyzed and compared to a unique significant database, which has been developed and is permanently updated by SoilCares' research team.

This world soil database consists of soil samples that have been taken from field studies all over the world and have been dried and shipped to SoilCares' Golden Standard Laboratory in Wageningen (the Netherlands).

In this laboratory the samples are analyzed both with traditional wet chemistry and with sensors and thereafter stored in the database. Spectra obtained from the Lab-in-a-box sensors are compared to the spectra in the database using intelligent software solutions and result in values of pH, macro- and micro-nutrients and customizable fertilizer advice.

The cooperation with PANalytical is of strategic importance to SoilCares. The Epsilon 1 XRF spectrometer meets all of SoilCares' specifications: it is very compact, able to quickly and precisely measure micro-nutrients and it is readily available.

SoilCares plans to target Ukraine, Russia, East Africa and the USA in the coming years and expects to sell at least 20 of their compact labs in 2016.

"Performing in a high-tech business as SoilCares is and developing game-changing products for new markets means that having reliable partners who understand our needs, are very important. We appreciate our cooperation with PANalytical and we are looking forward to a very positive future together."

- Robbert Ausems, international sales manager, SoilCares

SoilCares

SoilCares is an initiative of Dutch Sprouts holding, which aims to help farmers around the world to increase their yield by easy and affordable measuring and monitoring soil and crop quality.

SoilCares has developed easy-to-use soil testing solutions, accessible to all farmers. By combining the latest agricultural know-how with high-quality analytical experience and expertise the company aims to improve agricultural and horticultural procedures and thus increase the farmers' yields.

A team of 50 specialists, residing in Wageningen (the Netherlands), Nairobi (Kenya) and Istanbul (Turkey) is resolved to empower farmers all over the world.

Ready for a **new challenge**

Gjalt Kuiperes, recently installed PANalytical regional manager of the APAC region, about 'How to trust'

'How to trust' is the theme of this issue of X'Press. The first definition of 'trust' that comes up in a dictionary is: to believe in the reliability, truth, or ability of something or someone. The editors of X'Press have asked Gjalt Kuiperes for his opinion about 'trust'.

What would be your foremost feeling when you hear the word 'trust'?
I think trust is very commonly used in the day-to-day practice. The way I like to look at it is more from a 'reliable, counting on' perspective. What I try to say is that obviously trust is that you put matters in someone's hand and that you have confidence/certainty it will be done as discussed. But it is not only an individual in which you can/will have trust, it can be a government, an organization or a company.

Can you explain us how PANalytical contributes to 'trust'?
When you look at a company there are many different angles, the one from the customer of that company, the employee, the 'owner/stakeholders' etc. An employee trusts the company if the company treats the employees fairly in all aspects, such as promotion, remuneration or praise.
The employee can only trust the company if the company trusts the employee. If this mutual relationship of trust is there, it means that the company as a total, by means of the sum of all contributions of its individual employees, focuses on the right things.

I think our customers realize that PANalytical is doing exactly this. The worker in the factory does his/her job to ensure that the to-be-delivered solutions are up to par with the highest standards defined, whereas Logistics ensures on-time delivery and Service carries out the installation up to the expectations of the customer.

But I am not only talking about the execution of a task. Trust actually starts with the basic principles we as employees have all agreed to and adhere to in the strictest sense of the word. They are the central theme in all we do, be it business negotiations, resolving customer questions, designing new innovative solutions, handling competitive situations always keeping the (potential) customer's interest in mind.
PANalytical and its employees have done an outstanding job in having these thoughts embedded in all our actions. In the end it is all summarized in PANalytical's values which we live by heart and they serve as a compass for all our activities.

Do you have an example for PANalytical's contribution to 'trust'?
There are quite a few, actually. The infamous milk powder scandal, where 'poisonous' material was added to allow more manufacturers' profit, comes immediately to my mind. By using our solutions you can reliably control the quality of the milk powder for most elements and thus get to know whether it can be consumed.

I am also thinking of the iron & steel production where XRF and to a certain extent XRD contribute to control the quality of the steel produced, might it be a high-alloy steel, a low-alloy steel or a cast iron. It is obviously very important that all requirements for the applications of a particular steel are met and that you can trust its quality.

Another example is the cement production with its impact on the environment. Both XRF and XRD are used for quality control of clinker and cement. There are many new regulations regarding the CO_2 footprint and for that reason cement manufacturers are looking for alternative ways of producing cement. First of all they try to improve the kiln control by using XRD to analyze free lime. This is a measure to optimize the kiln and get the best results both product-wise as well as environmentally. Secondly, cement manufacturers try to substitute clinker (the product of the kiln) by additives to achieve the same end product (cement). These additives can be analyzed by XRD and the addition process can of course also be controlled by XRD.
These efforts result in a smaller CO_2 footprint of cement production and subsequently less impact on the environment. I think the examples I named illustrate the important role PANalytical can play in all aspects of a production process.

I have worked almost my whole professional life for PANalytical (formerly Philips Analytical). If you read the above you can perhaps imagine why so many people are working for so long with this company. PANalytical takes care of its people, our people take care of the needs in the market and are there to help and support our customers (in many cases 24/7). At the same time our products and solutions are contributing to a better world so who does not want to work for a company like that? Besides that, and that is more a personal preference, I love the world of process control, research/academia and the people working in these industries.

You have recently moved from the Americas to the APAC region. Are there special issues in the APAC region, different from the ones in the Americas?
That has literally been a move to the other side of the globe. Still the customers, with their needs and demands are not that different.

However, there is of course a huge cultural difference both of the customers and our employees. I am looking forward to understanding those differences and their meaning and it is a great challenge to adjust the style of leadership to get the most out of it for our people, our customers and our stakeholders.

Together as a team we tackle those challenges, adapt our behavior where needed, use best practices where possible and in the end keep a close eye on our employee and customer satisfaction.

"Trust actually starts with the basic principles we as employees have all agreed to and adhere to in the strictest sense of the word."

- Gjalt Kuiperes, regional manager PANalytical, APAC region

Gjalt Kuiperes graduated in Geology with a major in Petrology and Geophysics at the State University Utrecht Earth Sciences department. In 1989 he started as product manager XRF at Philips Analytical in Almelo, the Netherlands. After 6 years he moved to China as business manager of Philips China and in 1998 became regional director of the Asian Pacific region for Philips Business Electronics Analytical X-ray.

After one year as marketing manager Philips Branded Monitors Chungli Taiwan Gjalt was appointed president of PANalytical Americas in 2001. In January 2016 he has started in his new function as president of PANalytical APAC and is now based in Shanghai, China.

Advanced X-ray analysis for **Hetero Drugs Limited** R&D center

Hetero, a research-driven pharmaceutical company, is committed to the development, manufacturing and marketing of active pharmaceutical ingredients (APIs), intermediates and finished dosages. Today, Hetero is recognized as a world leader in process chemistry, API manufacturing, formulation development, manufacturing and commercialization.

Hetero has around 18 state-of-the-art manufacturing facilities, which are cGMP-compliant and have been approved by various Ministries of Health and regulatory authorities like US FDA, WHO, MCC (South Africa), MHRA (UK), TGA (Australia), PMDA (Japan) and KFDA (Korea). The company has a large product portfolio of over 200 products across a wide range of therapeutic categories.

Hetero has a strong global presence in over 120 countries and has been offering API's and generic formulations to partners across the globe. While Hetero is committed towards leveraging its expertise in the area of pharmaceuticals, it is also focusing on biotechnology and on developing new chemical entities (NCEs) in select therapeutic areas.

A state-of-the-art R&D facility of the company headed by director Dr. Kura Ratnakar Reddy is located at its headquarters in Hyderabad, India. Here 500 scientists are working on the development of generic drugs and new chemical entities. A large analytical lab, headed by Dr. Mamilla Yogeshwar Reddy, comprises all types of instruments for the analysis of pharma samples.

Precise characterization of the products is of utmost importance in the pharmaceutical industry. A slight variation of the molecular structure (polymorphism) can result in very different effects of a drug.
X-ray diffraction (XRD) helps to identify such differences in a non-destructive way. To check the presence of toxic elements in any drug, X-ray fluorescence (XRF) spectrometry is the method of choice as it is fast, reproducible, reliable and adopted by USP chapter <735>.

While the Hetero Group has been using these methods for many years, the latest advancements in analytical solutions have prompted them to go for a PANalytical Empyrean X-ray diffractometer. Its Bragg-Brentano^{HD} high-definition optics along with exchangeable Soller slits provide better peak symmetry, while implementation of an elliptical mirror yields reproducible high-intensity diffraction data. Additionally an *in situ* slurry flow cell enables on-line monitoring of polymorph growth. The PIXcel detector offers the highest sensitivity and excellent resolution and an Anton Paar CHC Cryo & Humidity Chamber helps with non-ambient *in situ* measurements.

Quantitative estimation of heavy elements in some of their drugs with XRF spectrometry has also come up as a recommended complementary technique for elemental analysis under USP chapter <735>. Compared to earlier techniques like AAS or ICP-MS, XRF stands out as the most convenient method as there is hardly any requirement of sample preparation and no need for additional chemicals.
As Hetero Drugs Limited is convinced of the superior analytical results they decided to be the pioneer institution to use XRF as its analytical tool in the Indian pharmaceutical industry.

"A slight variation of the molecular structure (polymorphism) can result in very different effects of a drug. X-ray diffraction (XRD) helps to identify such differences."

- Dr. Mamilla Yogeshwar Reddy, Associate Vice President Analytical Research and Development

Hetero is one of India's leading generic pharmaceutical companies and is the world's largest global producer of anti-retroviral drugs for the treatment of HIV/AIDS. Founded in 1993 by Dr. BPS Reddy, Hetero has grown rapidly in over two decades, based on a tradition of excellence, a strong-minded focus on cost-effective integration and with a deep sense of commitment towards making life-saving medicines accessible to patients worldwide.

Hetero, a privately-owned company, is recognized as one of the top 10 companies in the Indian pharmaceutical industry with an annual turnover of US$ 1.2 billion. With a dedication and support of its 15,000 employees, Hetero continues its commitment to manufacture high-quality drugs and save millions of lives across the world.

LeNeo® fusion instrument proves effective to prepare fuel oil for ICP analysis

Contaminants in fuel oil such as nickel, iron, vanadium, silicon, aluminium, sodium and calcium can cause corrosion in boilers and fuel engines. It is therefore important to accurately and reproducibly determine their concentrations.

Claisse released a new application note regarding the dissolution of fuel oil using borate fusion for inductively coupled plasma optical emission spectrometry (ICP-OES) analysis in accordance with ASTM D 5184, IP 377 and IP 501. These standards are used to specify the analysis of fuel oil by ICP-OES.

The use of a reliable instrument such as LeNeo® Claisse Fluxer® combined with an appropriate flux allows meeting the accuracy, recovery and precision criteria of such internationally recognized standards.

The preparation method described in this application note is beneficial for all laboratories since it is quick, reproducible and does not require the use of harsh acids. “The whole fusion and dissolution process takes less than 15 minutes”, says Philippe Daigle, product manager at Claisse.

The entire application note is now available on www.claisse.com/expertise.php where you can find more publications about XRF and ICP analysis.

PANalytical’s **Remote Assistance Suite** Always in control of your Axios/ Zetium system

For owners of PANalytical’s Axios and Zetium X-ray fluorescence (XRF) spectrometers the newest generation of secure and easy remote support solutions is now available. With this fast and efficient tool, help from our team is just a few clicks away.

The new Remote Assistance Suite comprises remote hard- and software support as well as support with your applications. If you need help you simply start our remote desktop tool to establish a completely secure connection from your system to our specialist. Each session is initiated with a one-time password and fully encrypted.

Additionally the Remote Assistance Suite offers a System Health Evaluator and System Certification for an evaluation of your system’s performance. With the help of our specialists you quickly know whether your system is working in peak condition. The Remote Assistance Suite comes with Super Q 5.3 for Axios systems and from Super Q 6.0F for Zetium systems. Both software versions are Windows 10 compliant. All systems with Super Q version 4.0 or higher can be upgraded to benefit from the Remote Assistance Suite features.

Contact your local representative for your personal software upgrade.

Easy and secure

Control and transparency

Always available

Events calendar 2016

The list shows a selection of events during the next few months where you will find us. Please come by and visit us when you attend any of these events.

29 March – 1 April	MRS Spring	Phoenix, AZ, USA
30 – 31 March	Forum Labo	Lyon, France
4 – 7 April	BCA Annual Meeting	Nottingham, UK
15 – 19 May	IEEE – IAS/PCA	Dallas, TX, USA

www.panalytical.com/events

PANalytical webinars

17 March	High-resolution diffraction – Exploration of the reciprocal space with high speed
7 April	Modern XRF equipment for cement processing
14 April	XRF theory in application – Which technology is better, WD or ED?
19 May	*In situ / in operando* XRD characterization of lithium-ion batteries

www.panalytical.com/webinars

50th anniversary of the **Rietveld method**

Exactly 50 years ago the Dutch researcher Hugo Rietveld (born in 1932 in The Hague) presented a new approach to structure refinement from powder diffraction data at the seventh Congress of the International Union of Crystallography (IUCr) in Moscow in 1966. The paper, titled 'Line profiles of neutron powder-diffraction peaks for structure refinement' was published in Acta Cryst. in 1967.

Rietveld originally worked with neutron diffraction data obtained from the research reactor at Petten (the Netherlands). His method was generally accepted only in 1977 when it was applied to X-ray diffraction data too. In that year the Commission on Powder Diffraction of the IUCr named the method after the author of the first publication. It took another ten years before people realized that the method can also be used for quantitative phase analysis, leading to a huge increase in popularity.

In the Rietveld method the entire diffraction pattern is taken into account, not just the intensities of diffraction peaks. By comparing measured and calculated diffraction patterns, a crystal structure model can be refined and the composition of a sample can be quantified.

Nowadays Rietveld refinements (and derived methods) are widely applied for routine quantification of crystalline materials in science and production control (e.g. for cement or steel making) as well as for the analysis of crystal structures.
The method is implemented in the Plus module of PANalytical's HighScore powder diffraction analysis software.

Colophon

Please send your contributions, suggestions and comments to the following address.

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For the analysis of fertilizers, soils, rocks and minerals

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Epsilon 3X, XLE

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