CPACT News

CENTRE FOR PROCESS ANALYTICS AND CONTROL TECHNOLOGY

August 2017

CPACT TEAM

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MEMBERSHIP

CPACT is delighted to welcome the University of Bremen to CPACT

The Technische Thermodynamik division at the University of Bremen is offering a unique breadth and diversity in applied spectroscopy. They have expertise in a large variety of optical and spectroscopic methods that allow a comprehensive characterisation of a given material or process. The techniques include vibrational spectroscopy (Raman and IR), absorption spectroscopy (UV, visible, Near Infrared), dynamic light scattering, fluorescence spectroscopy, non-linear optical methods (CARS, LIGS), and others. In addition, they develop and apply methods for data processing and evaluation including chemometrics, complex shearlets, etc.

Johannes Kiefer said "process analytics and control technology is the key for operating processes efficiently and environmentally friendly. As a member of CPACT, we are part of a unique multidisciplinary and international network. Together with our partners in academia and industry we are working for a sustainable future".

Everyone at CPACT is looking forward to working with Johannes and his colleagues at the University of Bremen.

SUCCESS OF THE BAYESIAN WORKSHOP

A half day workshop entitled 'Bayesian Statistics to Industrial Data' took place at the University of Newcastle on Thursday 18th May 2017.

Industrialists and researchers within CPACT have been exploring the application of Bayesian statistics to industrial data and processes. Generally, in the process industries and other sectors, a frequentist (or traditional) approach to statistical analysis is applied within methodologies such as statistical process control (SPC), design of experiments (DoE) and capability analysis. There are significant benefits in using a Bayesian approach such as:

- the incorporation of expert industrial/process knowledge into analyses
- the ability to combine effectively statistical analysis with decision support
- an understanding of all of the elements of uncertainty in a problem

Delegates from GSK, BP, Fujifilm, Centre for Process Innovation (CPI), Johnson Matthey and Newcastle University gained an understanding of Bayesian principles and worked through capability analysis examples directly comparing the frequentist and Bayesian approaches. The workshop concluded with a discussion on relevance and applicability to delegate organisations. Requests were made to develop further workshops with a primary focus on DoE and SPC.

Newcastle University academics are keen to identify collaborative industrial research partners in this area - please contact Matthew.Linsley@newcastle.ac.uk if you are interested in discussing this further. Newcastle University is also keen to gauge demand for the potential development of software to conduct Bayesian analyses in process contexts.

For more information about CPACT, link to our FACTSHEETS:

CPACT NETWORK

RESEARCH AT CPACT

MEMBERSHIP BENEFITS

CPACT'S ACHIEVEMENTS

BUSINESS BENEFITS OF PROCESS ANALYSIS & CONTROL

CPACT EVENTS

www.cpact.com

CPACT CELEBRATES 20 YEARS!
4-5 October 2017, University of Strathclyde, Glasgow

CPACT will celebrate 20 years since its beginning in 1997 which probably makes it the longest running UK-based centre of its type! We have now finalised an exciting two day scientific programme which will portray a glimpse of CPACT from past, present and future perspectives.

There will also be a celebration dinner in the evening of 4th October at the Corinthian Club in Glasgow. To view the scientific programme and to register click here::

http://www.cpact.com/events/research/20171004_cpacts_20th_anniversary_event

PROCESS SPECTROSCOPY COURSE
16-18 January 2018, Clairet Scientific, Northampton

Process Analysis is an integral part of process optimisation, process control and performance monitoring. Rapid analytical measurements are increasingly required in industry to monitor progress of a reaction, know when the end-point of a process has been reached, check reaction kinetics, detect impurities or control blending, granulation, etc. All these activities and many more require timely qualitative and quantitative information. This can often be provided through at-line, on-line, in-line or non-invasive application of molecular spectroscopy techniques. The course provides an introduction to molecular spectroscopy through a series of presentations and practical exercises/demonstrations on process spectroscopy techniques, including NIR, MIR, UV-visible, Raman spectrometries. Developments in complementary process analysis procedures based on light induced fluorescence spectrometry, mass spectrometry, NMR spectroscopy and acoustic measurements will also be described. Emphasis will be given to the practical application of spectroscopy to process analysis.

Further details: http://www.cpact.com/events/courses/20180116_process_spectroscopy_course

APACT — 25-27 April 2018
Newcastle, UK

APACT is an open forum for the presentation and discussion of recent scientific and engineering advances relevant to process analytics and control technologies. Plenary and keynote speakers will report recent advances in the development and application of novel process analytics, predictive modelling and control technologies, and will review the benefits achieved. Following the success of previous conferences, APACT 18 will be a 3 day meeting featuring plenary and parallel sessions on topics crucial to the achievement of manufacturing excellence.

Confirmed speakers are:

Thomas De Beer, Ghent University—Model based optimal process analyser implementation in pharmaceutical manufacturing processes
Lee Smith, Process Instruments—Raman applications throughout the petroleum refinery—crude unit to blending
Christoph Herwig, Technical University of Vienna—Multi-parametric control strategies for enabling continuous biomanufacturing
Tom Rodgers, The University of Manchester—Electrical tomography for on-line process monitoring
Vicki Woodward/Nicholas Pedge, AstraZeneca—Establishment and lifecycle management of transmission Raman spectroscopy for near-time monitoring
Chee Wee, ICES—Scaling up batch polymorphic crystallization using PAT/QbD approach
Sean Bermingham, PSE (ADDopT) - Digital design (and operation) of drug products and their manufacturing processes
Patrick Wray, Bristol-Myers Squibb—High speed video analysis and modelling as techniques for scale up of wet granulation

The event includes a poster session and exhibition. To secure your space, please contact admin@cpact.com. Further details: https://apact.co.uk/

Recent Webinars and company benefits

CPACT Webinars

Participation in CPACT webinars is free of charge for members making it an excellent training resource and benefit. Additionally, all webinars are recorded and can be accessed from the CPACT website (www.cpact.com members area).

Recent webinars include:

- Inspection of capsule filling led by Fabien Chuchard from Indatech (12 Jan 2017)
- Bayesian inference led by Malcolm Farrow from Newcastle University
- On-line elemental analysis led by Philip Martin from University of Manchester (9 Feb 2017)
- Software sensors and inferential estimation led by Jie Zhang from Newcastle University and Julian Morris from CPACT (16 Feb 2017)
- Mixing and/or blending of solids and liquids led by Richard Escott from Indatech (23 Feb 2017)
- Statistical analysis methods led by Matt Linsley from Newcastle University (webinar series March & April 2017)
- In-line Raman in real life biotech and industrial manufacturing led by Fabien Chauchard from Indatech (27 April 2017)
- Towards process monitoring using hyperpolarised NMR led by Peter Richardson from University of York (25 May 2017)
- Parameters in mathematical models and how to treat them: estimation, uncertainty and sensitivity led by Alex Kiparissides from UCL (8 June 2017)

Webinars are a huge benefit of CPACT membership — they are excellent training resources for companies and best of all they are free!

Upcoming Webinars

MULTISPECTRAL FIBRE SENSING FOR REMOTE PROCESS CONTROL
31 August 2017 AT 15:00 (UK time)
Slava Artyushenko, art photonics

A NOVEL CHALLENGE IN COMPLEX PROCESSING—THE IMPACT OF CO-INTEGRATION FOR DYNAMIC PROCESS PERFORMANCE MONITORING
2 November 2017 AT 15:00 (UK time)
Puneet Mishra and and Atakan Sahin, University of Strathclyde

FLUORESCENCE SUPPRESSION BY (INSTANTANEOUS) SHIFTED EXCITATION RAMAN DIFFERENCE SPECTROSCOPY
**30 November 2017 AT 15:00 (UK time)**
Johannes Kiefer, University of Bremen

FOR FURTHER DETAILS AND UPDATES VISIT: www.cpact.com

GSK feasibility study was a resounding success!

Venoruton: Raman as an alternate to off-line UV analysis

GSK Consumer Healthcare has manufactured Venoruton gel, a topical treatment for varicose veins for many years at Nyon in Switzerland. The process involves selective alkylation of the phenolic alcohol functionalities of natural product derived Rutin (Scheme 1). The target is to reach a specific percentage of hydroxylation and a specific mixture of hydroxylated species.
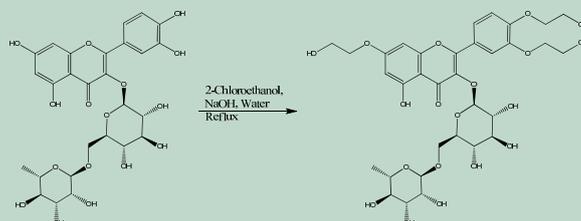
Scheme 1: Venoruton Gel and Reaction Chemistry

The specific mixture of hydroxylated species is registered and is a key function of the medicine's activity. Attaining this specific mix requires careful control of the reaction conditions and reaction stoichiometry. Achieving this mix is challenging and it is possible to exceed the degree of hydroxylation desired with minimal changes in reaction stoichiometry or minimal changes in the reaction conditions. Minor deviations have caused batches to be lost. The batch size is 1.5 tonnes so this can be a considerable financial loss and can impact the supply of this medicine to patients.

GSK engaged CPACT to investigate if there may be a process analytical solution to determining the reaction end point in real time and thus allowing an immediate quench and reducing significantly the risk of going beyond the desired endpoint. Scientists at the University of Strathclyde devised an excellent screening programme of a variety of analytical techniques to assess if there may be an in-line process solution. The techniques investigated in the study include Raman, near-infrared (NIR), mid-infrared (MIR), and nuclear magnetic resonance (NMR) spectroscopy. Samples were supplied by GSK of Rutin at various intermediate stages of hydroxylation.

Out of the spectroscopic techniques under investigation NIR, MIR, and NMR spectroscopy produced spectra that were found to be dominated by the signature of water present as a solvent in the aqueous samples. In contrast, Raman spectroscopic measurements in combination with a simple intensity ratio approach, showed potential as a straightforward process monitoring strategy.
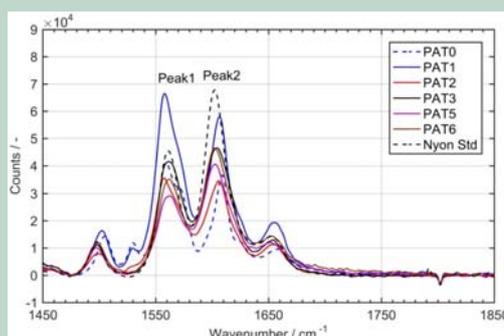

Figure 1: Raman spectra of Rutin samples supplied by GSK

Raman showed a clear differentiation as the reaction progressed (Figure 1) and appears to be a very promising lead to a potential in process reaction tracking method.

The next step in this study is for GSK to internally evaluate Raman in a 'live' reaction and further to assess the feasibility towards validation.

From a GSK perspective the interaction with CPACT has been a resounding success. A potential solution has been determined to a long standing process control issue. The technical capability and academic knowledge yields a resource that is quite unique in an area that is currently of very high interest to the pharmaceutical industry.

We would in GSK like to thank the scientists and staff who supported this work in particular Florian Zehentbauer, David Littlejohn, Alison Nordon, Andrew Parrott and Natalie Kerr.

3D Raman Hyperspectral Imaging
Clairet Scientific

As part of the feasibility study programme, Clairet Scientific will be supplying an H2OPTX 3D Raman Hyperspectral Imaging system on loan to CPACT this Autumn. The instrument generates 3D images from pharmaceutical tablets and similar sized objects, providing valuable insights into particle size distribution and chemical composition. It can also produce 2D images which can be extremely useful in examining samples such as complex powder mixtures, particle by particle.
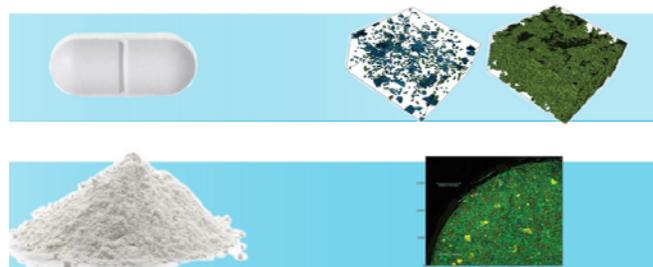
CPACT members wishing to have samples analysed should initially contact either Florian Zehentbauer at Strathclyde or John Andrews at Clairet Scientific. Any work done for Members can be covered under the confidentiality clauses of the CPACT Membership Agreement.

CPACT Technical Director visits BP Hull

Inferential sensing (also known as soft sensing or virtual sensing) is a powerful and increasingly used methodology that allows process quality, or a difficult to measure process parameter, to be inferred from other easily made plant measurements such as pressure, flow, temperature, etc. Inferential sensing finds application in a wide range of industries including petrochemical, refining, oil/gas, biofuels, pharmaceuticals etc. However BP considered that inferential sensing was underutilised in its businesses and that an opportunity existed to make better use of this modelling technique.

In November 2016 a workshop was held at BP Chemicals Hull site to discuss inferential sensing theory and application. Around 30 people attended the workshop including process engineers, chemists, automation engineers, managers and plant optimisation engineers. The workshop consisted of three technical sessions, punctuated with a live demonstration of the CPACT PreScreen software and followed by a discussion session. The technical sessions were presented by Julian Morris (Technical Director, CPACT), Sean Goodhart (Principal Engineer – Control and Automation, BP) and Mark Evans (Advanced Control Engineer, BP Hull).

Julian Morris provided an introduction to the concepts of inferential sensing and some of the potential pitfalls before moving on to give an external expert view on opportunities for inferential sensing and providing case studies on the use of inferential sensing in other industries. Julian also discussed some of the more advanced techniques available to help develop inferential sensors.

Sean Goodhart described the technical approaches used to develop inferential sensors, providing examples where inferential sensing is currently used within BP and describing the tools available for building inferential sensors. Sean also provided further theory on variable selection and then compared abstract versus first principle modelling techniques and discussed the relative merits of both. He then provided a walkthough of the preferred software package used by BP along with handy tips on how to process data.

Finally Mark Evans described an inferential sensing application being developed at BP Hull, the methodology he used to develop the application and how he deployed the application. Mark then presented validation data against offline measurements as well as discussing opportunities for future improvement.

Julian Morris also gave a live demonstration of the CPACT PreScreen software using example datasets to highlight the use of this powerful tool for screening and gaining insight from process data.

The following day Julian Morris provided expert consultancy on 2 specific process challenges. During these sessions the PreScreen software was further utilised to explore process data and gain insight.

The feedback received from attendees was very positive. Attendee's knowledge of inferential sensing has been increased and this technique can now be considered for application at all scales of process where measurement challenges exist. A wider review of candidate applications for inferential sensing at the BP Chemicals Hull site has begun and applications will be further developed throughout 2017. After the workshop a number of attendees have requested access to the PreScreen software and now use the software in their routine data analysis workflow. Based on the use of this software BP has been able to suggest a number of additions to help improve the PreScreen software in the future. Julian's attendance at this workshop was kindly funded via the CPACT feasibility study program.

Craig Herdsman, Analytical Chemist, BP Chemicals.

REMINDER - FUNDING OPPORTUNITIES

SUPPORT FOR BID WRITING

CPACT is dedicated to the development and application of process analytics and control technology.

Many of the national and international calls for research proposals, such as innovate UK, BIS and Horizon 2020, involve considerable time and effort on the behalf of industrial and academic partners, at a very early stage of the bid process. Often, the deadline for submission to calls is extremely short, which challenges the resource availability to complete them.

CPACT wishes to remove barriers to participation in these calls, to increase the research effort in process analytics and control technology. To that end CPACT is offering funds to support the utilisation of professional bid writing, to ease the strain on potential partners and improve the chance of successful application.

For stage one applications, this will normally be limited to a contribution to costs of £1K with up to £5K for stage 2.
Applications should be for projects with themes in areas of interest to CPACT members: http://www.cpact.com/research/projects/current

In the first instance, interest should be directed to admin@cpact.com

SUPPORT FOR STUDENTSHIPS

CPACT is keen to encourage and enable researchers to leverage university/CASE/industrial funding to support PhD studentships in areas of interest to CPACT members.

To that end, CPACT is offering 5 x £10k bursaries, offered as a contribution to the costs of new PhD studentships.

If you are interested in this funding, please contact us for further information and application guidelines: admin@cpact.com

CPACT MEMBERS EXHIBIT IN POTSDAM

The EuroPACT conference took place in Potsdam, Berlin on 10-12 May 2017.

EuroPACT 2017 was the fourth European Conference on Process Analytics and Control Technology. The conference covered new technologies in process analytics, the implementation of these technologies in various fields and the transformation of data into knowledge. The conference was supported by 20 exhibitors of instrumentation, applications and data evaluation tools. Seven of the CPACT member companies exhibited at this event; art photonics, CAMO Software, Hellma, Keit Spectrometers, Indatech, Polytec and tec5. A total of 220 delegates attended from countries all over the world and the conference was a huge success. The next EuroPACT conference will take place in 2020 and further details will be advertised in due course.