

CPACT TEAM



Natalie Kerr
Administration Manager
(currently on maternity leave)



Carol Badger (covering)
Administration Manager
CPACT Strathclyde
E: carol.badger@strath.ac.uk
T: 0141 548 4836



Christine Stevenson
Administrator
CPACT Strathclyde
E: christine.stevenson@strath.ac.uk
T: 0141 548 4787



Julian Morris
CPACT Technical Director
E: julian.morris@strath.ac.uk

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CENTRE FOR PROCESS ANALYTICS AND CONTROL TECHNOLOGY

News

July 2016

Membership: Who's new?

CPACT is delighted to welcome several new members to the network.

END USER



DSM Resolve

DSM Resolve is part of Royal DSM N.V., a global science-based company active in health, nutrition and materials. This branch of the company acts as a high end analytical solution provider with a key interest in linking process design to process control in a manufacturing environment by means of a process analytical strategy.

They believe that by combining best practices with other CPACT members, they can become an active partner, working together to tackle analytical challenges and provided innovative and sustainable solutions.

EARLY-STAGE RESEARCHER FEASIBILITY STUDIES

CPACT is looking to extend its highly successful feasibility study programme by soliciting proposals from early-stage researchers within the CPACT academic partners.

Successful proposals will be awarded £5k to undertake a short feasibility study. Further details including criteria for proposals and submission form can be found at www.cpact.com

Forms should be completed and returned to Carol.badger@strath.ac.uk
The first call deadline is 31st August 2016.

The project outcomes will be presented at a CPACT research day and/or the APACT conference following completion of the study.

SME

Thomas Swan & Co. Ltd:

The company is a leading independent manufacturer of performance and speciality chemicals. Internationally recognised for innovations in chemical manufacturing, they believe that sharing their experience will be beneficial to members who would like to collaborate on the novel development of creative, cost-effective solutions.

The company hopes to gain exposure to "state of the art" novel Process Analytics innovations and learn from the knowledge of members of CPACT.



RESEARCH INSTITUTE

Institute of Research and Agrifood Technology

(IRTA):

IRTA is a public research institution, part of the Department of Agriculture, Food and Rural Action of the regional Government of Catalonia, Spain.

IRTA's mission is to contribute to the fostering of sustainable development in the sectors of agriculture, animal and plant production, food technology and aquaculture.

Through CPACT, they aim to collaborate with partners from other sectors (e.g. chemical, pharma) and develop innovative research projects, implementing novel sensor technologies.



UNIVERSITY



University of York:

A member of the elite Russell Group of universities, York is a dynamic, research-intensive university committed to the development of life-saving discoveries and new technologies. The university brings expertise in a wide range of analytical techniques and methods together with extensive experience of industrial collaboration.

It hopes to engage proactively with industry, contributing strength in a range of spectroscopic and other analytical methods embedded in its Chemistry, Physics and Biology Departments, with Mathematics and Computer Science contributing through embedded systems and data analysis.



University College London:

UCL is one of the world's leading universities for research excellence. UCL has extensive research and training facilities including the interdisciplinary Advanced Centre for Biochemical Engineering. It has a close working relationship with industry providing unparalleled opportunities for research teams to tackle long term problems with leaders in the sector.

The university also brings one of the largest and strongest Statistics departments in the UK, with a wide range of research interests, both methodological and applied.

WHY JOIN CPACT? - KEY BENEFITS

CPACT advances manufacturing excellence to deliver business benefits across all sectors of the processing and manufacturing industries

CPACT initiates leading edge R&D and technology transfer for the exploitation of process analytics and control technologies

CPACT is managed by its industrial and academic partners with support from the Knowledge Transfer Network

BUSINESS IS BASED UPON SUSTAINABLE PROFITABILITY:

PROCESS ANALYSIS AND CONTROL BOOSTS YOUR BOTTOM LINE

www.cpact.com

CPACT

For detailed information on CPACT, fact sheets are available on our website: www.cpact.com

Below is a summary of the benefits that members may enjoy:

- ◆ Access to expertise with over 30 industrial member companies, 8 universities and 2 research institutes.
- ◆ Meet strategic company goals through participating in specific Research Council, TSB and EU projects
- ◆ One-stop shop for implementation support in process analysis and control technologies
- ◆ Proven business benefits from knowledge and technology transfer
- ◆ Involvement in a forum raising the profile of process analytics and control technologies across all process, chemical and pharma sectors
- ◆ CPACT Collaboration Agreement allows easy collaboration with members with no confidentiality concerns



- ◆ World-wide networking with major process and pharma companies, technology vendors and academia
- ◆ Free webinars and subsidised attendance at conferences, Continuing Professional Development and applied learning courses
- ◆ APACT conference - discounted attendance fees and free exhibition space for members
- ◆ Shared learning and benefits through Open Innovation
- ◆ Recruit and have access to highly skilled PhD students and Post Doctoral graduates
- ◆ Free CPACT Software Toolboxes:
 - User friendly data visualisation and pre-processing
 - Multivariate data analysis and modelling
 - Design of experiments and optimisation
- ◆ Member access to free short term feasibility studies into process analysis and control applications



CPACT EVENTS

FORTHCOMING EVENTS

14 September 2016

CPACT Research Day
University of Strathclyde
09:30-16:30

15 September 2016

Steering Committee
University of Strathclyde
09:00-15:00

17-19 January 2017

Process Spectroscopy
Course
Clairet Scientific Ltd.
Northampton
Details:
http://www.cpect.com/events/courses/20170117_process_spec_troscopy_course

10-12 May 2017

EuroPACT 2017
Potsdam, Near Berlin
Details:
<http://dechema.de/en/europact17.html>

www.cpect.com

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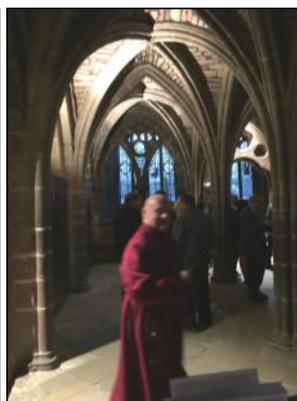
The Crowne Plaza Hotel, Chester was the venue for this year's APACT and, once again, the conference was rated as highly successful with a strong line-up of internationally renowned plenary and keynote speakers. Special thanks to all the presenters from both UK and international locations who delivered excellent presentations and whose contributions were much appreciated.

Three pre-conference courses were offered and these were very well received by participants:

- Introduction to Process Control
- Introduction to Chemometrics
- Classical Least Square Methods/ Multi-block, Multi-set, Multi-level and Data Fusion Methods

Social activities were also enjoyed with a reception and tour of Chester Cathedral (after an escorted walk by some Roman soldiers!) in the evening of day 1, and a conference dinner and casino event at the Crowne Plaza Hotel following the programme on day 2.

However, it was clear from feedback that the highlight of the conference was the unique Exhibitors' Showcase which took place in two parts and featured short presentations by the vendor companies who participated in the conference exhibition. The showcase chairman, David Littlejohn, provided a humorous lead to the sessions, and the contributors followed suit, catching the spirit of the show and making it entertaining and memorable! A bottle of champagne was awarded to the best showcase which this year was won by Siemens.



The poster exhibition was also well supported and provided an opportunity for both students and industrialists to present their work to a select audience. The poster prize, sponsored by Clairet Scientific, was awarded jointly to James Thomson, University of Manchester and Yehia Amar, University of Cambridge.

Also of note from the conference survey forms were comments regarding the special atmosphere which is prevalent at APACT conferences, making it a friendly and useful gathering of like-minded scientists and engineers, which not only informs and updates on advances in process analytics and control technologies, but also promotes excellent networking opportunities for users and vendors alike.

Next year our sister conference EuroPACT will be held at Potsdam, Germany (10-12 May 2017) <http://dechema.de/en/europact17.html> APACT will continue in 2018, details to be confirmed.



Left to right: Julian Morris, Sulaiman Lawal, Matt Linsley (who sponsored student attendance from his webinar honorarium), Newcastle University



Poster Prize winner: James Thomson, University of Manchester with sponsor John Andrews, Clairet Scientific Ltd.



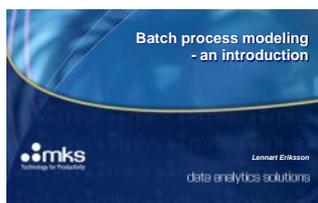
Poster Prize winner: Yehia Amar, University of Cambridge with John Andrews

Success stories

The webinars hosted by CPACT have gone from strength to strength recently with many more interesting topics planned for future months.

Recent sessions include:

- Batch Process Modelling lead by Lennart Eriksson from MKS Data Analytics Solutions in Jan 2016.



- Introduction to DoE — a series of 4 webinars led by Matt Linsley, Newcastle University in March/April 2016.



- Eigenvector — single webinar led by Barry Wise from Eigenvector Research Inc. on 31 May 2016.



INTRODUCTION TO CHEMOMETRICS (MULTIVARIATE ANALYSIS)

WEBINAR 1 - CHEMOMETRICS SERIES 2016
GEIR RUNE FLAATEN - CAMO SOFTWARE AS



- Introduction to Chemometrics (Multivariate Analysis) — a series of 6 webinars led by Geir Rune Flaaten, CAMO Software. This series completed on 8 June 2016.

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

Future Webinars

ATR FTIR Spectroscopic Imaging 8 July 2016

— will be led by Sergei Kazarian and Andrew Ewing, Imperial College London

This webinar presents recent developments of the use of ATR-FTIR spectroscopy and spectroscopic imaging to study the dissolution of tablets and monitor drug release in real-time. ATR-FTIR spectroscopic imaging can be employed to investigate drug release from tablets, revealing spatially resolved and chemically specific information about pharmaceutical systems. This reliable imaging approach has recently been adopted by industry where it is used as a method to assess the quality of formulations. An exciting future direction of ATR-FTIR imaging is to study the behaviour of pharmaceutical formulations in micro-fluidic channels. This can provide high-throughput information about the processes of drug release under flowing conditions.

On-line Elemental Analysis 6 October 2016

— will be led by Philip Martin, University of Manchester

Statistical Analysis Methods

— a series to be led by Matt Linsley, Newcastle University early in 2017.

Company Benefits

Companies should note that participation in CPACT webinars is included in the membership agreement at no additional cost, making it an excellent training resource and benefit.

Details of forthcoming webinars are publicised on the CPACT website and staff who wish to register should contact Christine Stevenson or email us at: admin@cpact.com We are always open to suggestions for new webinar topics and also welcome any member who has expertise in a particular area and would like to share with others. If this is you, please get in touch with us to discuss.

Finally, a big thank you to those who have previously contributed to the success of CPACT webinars. This is much appreciated by all and enhances our learning experience and sense of belonging to a specialised network.

CPACT has developed software tools that are available free to all member categories.

Links and instructions on downloading can be found on the members only site (password required).

www.cpack.com

Here you will find the latest software-related news; an overview of the different packages; a download section; a presentation/online help for PreScreen; and links to Matlab related websites.

COMING SOON!

SPECTRAL

SHOOTER:

Spectral Pre-processing,

Calibration

Maintenance and

Calibration Transfer toolbox.

This newly developed software is almost ready for testing and will be released very soon.

Data PreScreen

A Multivariate Statistical Data Pre-screening Toolbox (Pre-Screen) has been designed and developed for use by the practising process engineer who wishes to pre-process and pre-screen process data prior to multivariate data analysis, process data modelling or building predictive and inferential models. Currently all commercial data analysis packages address the univariate situation which is inappropriate in today's industrial environment. In this situation, a large number of highly collinear and noisy process variables are collected for use in process modelling or performance monitoring, and the initial data cleaning and conditioning task can consume up to 75% of the modelling time. A software toolkit has been developed specifically with the aim of focusing on the industrial needs for the initial data pre-screening of large data sets.

The core feature of **Pre-Screen** is that it has been specifically developed to make the analysis of large data sets as automated as possible without taking away the need for engineering science understanding. The toolbox builds on top of the MATLAB programming environment, with powerful user interface procedures providing user friendly, mouse/menu driven software. The Main Features of **Pre-Screen** include: Data Tags, Load and Save facilities, Data Plotting, Normality (Univariate and Multivariate), and Summary Statistics (mean, standard deviations, covariance, correlations, skewness and kurtosis), Missing Data analysis and rectification, Spurious (outlier) Data Elimination, Data Transformations, Data Filtering, Cross Correlation, Data Transformations (Mathematical and Time Shifting), Scatter Plots to Observe Possible Relationships, Loadings and Contribution plots, Histogram Plots, Normal Probability plots, Action tracking, and plot copying to WORD files.

MultiDAT

This Multivariate Data Analysis Toolbox (**MultiDAT**) is designed for the practising process engineer who wishes to analyse process data for plant data interpretation, feature detection and process modelling. The toolbox builds on top of the MATLAB programming environment, with powerful user interface procedures providing user friendly, mouse/menu driven software. The core feature of **MultiDAT** is that it has been specifically developed to analyse two data sets: a reference or nominal data set i.e. data collected when the process is in a state of statistical control where only common cause variation is present, and a second data set which is either a validation set (i.e. it has not been used in the development of the model) or alternatively, a data set which contains faults, typical of those found on the process.

The main features of **MultiDAT** include: editing functions, chronological log, and plotting functionality; Residual Analysis, Contribution Analysis, Regression Coefficients, R^2 and R^2 -adjusted, Cross Validation Modelling Methodologies; Multiple Linear Regression (MLR) or Ordinary Least Squares (OLS), Stepwise Regression, Principal Component Regression (PCR), Projection to Latent Structures or Partial Least Squares modelling (PLS); Multivariate Statistical Process Control – MSPC (Process Performance Monitoring): PCA based monitoring, PLS based monitoring; exporting data, graphs and pictures to any Windows Application.

BatchDAT

This Multivariate Statistical Modelling and Batch Statistical Process Control Toolbox is designed for the practising process engineer who wishes to analyse batch process data for plant data interpretation, feature detection and process modelling. The toolbox builds on top of the MATLAB programming environment, with powerful user interface procedures providing user friendly, mouse/menu driven software. The core feature of **BatchDAT** is that it has been specifically developed to analyse batch data by two routes: (i) through-batch observation level – (Wold et al. - Method 1) and (ii) between-batch comparison level – (Nomikos & MacGregor - Method 2). The Main Features of **BatchDAT** include: Load and Save facilities, Data Plotting and Descriptive Statistics, Trend Plots, Histogram and Normal Probability Plots; Three-way batch data unfolding for: (i) through batch observation analysis and (ii) between-batch analysis for comparisons between batches; Principal Component Analysis (PCA), Multi-way PCA and Multi-way PLS monitoring, Batch Loadings and Contribution plots, Action tracking, and Plot copying to WORD files.

NewNet

This Neural network modelling toolbox (**NewNet**) has been designed and developed for use by the practising process engineers who wish to build nonlinear models using industrial process data for process predictive modelling, inferential estimation and software sensors. The Main Features of **NewNet** include: Static and Dynamic Neural Networks, Building Network Models from Minimal Data, Network Stacking for Robustness, and Model Validation.

DoEMan

The **DoEMan** software allows the use of a design of experiments (DoE) approach to building a calibration model in an unbiased manner. The output of the DoE can be viewed graphically and interrogated to assist identification of the most appropriate data preprocessing techniques. **DoEMan** forms a useful tool for those using the PLS Toolbox in the MATLAB environment.

NEW RESEARCHERS

CPACT is delighted to welcome three new researchers who have joined us to work on an EPSRC funded project entitled “A paradigm shift in low-field NMR spectroscopy for industrial monitoring, control and optimisation.”

This project is a collaboration between Prof Simon Duckett and Dr Meghan Halse (University of York) and Dr Alison Nordon (University of Strathclyde) and includes support from industrial partners including the Centre for Process Innovation Ltd., Domino UK Ltd., GlaxoSmithKline, and Pfizer.

Andrew Parrott joined us at University of Strathclyde in February 2016.

Nuclear Magnetic Resonance (NMR) spectroscopy, a powerful laboratory-based technique, has had limited application for *in situ* process analysis. The aim of this project is to develop a low cost, low-field NMR instrument for process monitoring, control and optimisation with the specificity of high-field NMR and enhanced sensitivity.

It is hoped that the project will be successful in opening up new opportunities for on-line NMR spectroscopy for process monitoring, control and optimisation. This will enable compositional monitoring not only of bulk components, but also tract level detection in liquid processes, where there is currently a significant measurement gap for a wide range of industries and processes from conventional batch to novel intensified and continuous manufacturing.



Andrew Parrott,
University of Strathclyde



Peter Richardson
University of York

Peter Richardson also joined us as a Postdoctoral Research Associate on the project and is based at University of York.

Peter's current research is focused on the development of a low-field (1 T) NMR instrument to be used for process monitoring, control and optimisation, with the aim of achieving the sensitivity and specificity of a high-field (ca. 10 T) spectrometer with the use of para-hydrogen induced hyperpolarisation.

His research is split into two parts, firstly, development of a bespoke polarisation delivery system for *in situ* hydrogenation of samples using para-hydrogen and secondly, identifying industrially and academically useful reactions which can be monitored using this method of hyperpolarisation.

We are also happy to introduce PhD student, Olga Semenova (University of York), who similarly links into this project.

Olga's research concerns the development of low-field NMR instrumentation for industrial use. She will seek to apply low-field (1 T) NMR to simple reactions like esterification. The cutting-edge technique SABRE (Signal Amplification by Reversible Exchange) will be applied in order to increase the sensitivity of the low-field NMR method. SABRE uses iridium complexes to catalytically transfer polarisation from para-hydrogen to a substrate molecule.

In further research, Olga will seek to broaden the range of reactions that could be monitored online in industry by specialists and non-specialists using benchtop low-field NMR with a flow system.



Olga Semenova
University of York