

CENTRE FOR PROCESS ANALYTICS AND CONTROL TECHNOLOGIES

CPACT NEWSLETTER

November 2010

CPACT COMPANY IMB REPRESENTATIVES

Members are reminded to contact their CPACT IMB representative if they have any general questions start up.

your company is listed below:

AJM Consulting - Alan Mason **BP** - Craig Herdsman **CAMO Software - Frank Westad** Clairet Scientific - John Andrews **CPI** - Chris Dowle Fibre Photonics - Gary Colquhoun Fujifilm - Colin Robertson Genzyme - Bob Samuel GlaxoSmithKline - Paul Slavin Infineum - Michael Minotti Johnson Matthey - Peter Ash MKS Instruments - Tim Robinson **National Nuclear Laboratory - Colin** Clarke

Perceptive Engineering - David Lovett

Pfizer - Mojgan Moshgbar Syngenta - Peter Oggenfuss

PFIZER RE-JOIN CPACT

Pfizer have recently re-joined CPACT as they are interested in general research being conducted by academic partners in CPACT in the areas of biologics, and Advanced Process Control.

David Littlejohn has a new role!

about CPACT or if they have any Professor David Littlejohn, currently one of the project ideas that they would like to CPACT Directors, has been appointed as Associate Deputy Principal to assist the new Deputy Principal for Research and Knowledge Exchange The current IMB representative for in Strathclyde's preparations for the Research Excellence Framework.

> Professor Littlejohn's excellent research credentials, combined with his senior management experience, will contribute strongly to the University's development. He officially started his new post on 1 August 2010.

CPACT participate in EXPO 2010

This event, which took place on 2nd November 2010 at the Science Centre in Glasgow, presented an exciting opportunity for business people, policy makers and 3rd sector organisations to access the latest cutting edge research from Strathclyde academics.



CPACT had a joint stand with the P&A Chemistry Department from Strathclyde University. David Littlejohn chaired a well attended discussion session on the proposed multi-university centre for continuous manufacturing and crystallization that will be housed at Strathclyde (more info about this on page 2).

CPACT TEAM



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Knowledge Transfer Partnership update

I am now into the second year of my Knowledge Transfer Partnership (KTP) between Newcastle University and the National Nuclear Laboratory/Sellafield Ltd. The aim of the project is to develop multivariate statistical predictive models and process performance monitoring tools in Waste Vitrification Plants.

The project is going well with a process performance monitoring tool being in the validation stage. Further offline testing is due to be carried out over the next few weeks, before online testing occurs. A number of

different issues have been highlighted which need more complex data analysis methods. Therefore, we are highlighting to plant staff that the KTP is benefiting them also. One of these is to determine which swabbing strategy is statistically better to remove contamination. This could be a large benefit to operations as it is a bottleneck of the process. If the best strategy is determined then there is a likelihood the number of swabs needed will be reduced and hence in the same time, more containers can be processed.

Recently, I attended a Knowledge Transfer Partnership Showcase night at the Hilton in Gateshead with my University supervisors Dr. Jie Zhang and Prof. Julian Morris, with other Associates highlighting the benefits that the project had given the company, university and themselves. It was a good opportunity to gain contacts across the North East and highlight the benefits that have occurred already. I produced a poster emphasising the three-way benefits. Next year, I will be giving a 2 minute pitch on the benefits that my KTP project has had; with the opportunity to win a prize.



Katy Ferguson CPACT Newcastle/NNL/Sellafield Ltd

Shaken not Stirred: SPIRIT Collaboration in Crystallisation Science part of the CMAC (Continuous Manufacturing and Crystallisation) Consortium

The CMAC-SPIRIT Crystallisation Science consortium is a new multi-centred research programme funded under the Scottish Funding Council's SPIRIT Scheme, in partnership with industry and the participating Universities. Among other initiatives, this Consortium establishes a "mini-DTC" comprising nine fully funded studentships across Glasgow, Edinburgh, Heriot-Watt and Strathclyde Universities, together with pilot nodes using continuous crystallisation technologies, aimed at delivering underpinning academic solutions to real industrial end-user problems. The project is part of a new collaborative initiative to develop novel technologies for continuous manufacturing and crystallisation in industry.

In many crystallisation processes, batch based solutions are adopted by default, in spite of the fact that they may not be optimised for the process. Although development of new process platforms can have major economic and environmental impacts, and continuous crystallisation has been increasingly a focus of attention in the pharmaceutical and other industries, investigations of such systems have not been widely carried out. The CMAC-SPIRIT project will examine both fundamental and applied aspects of nucleation and crystallisation processes underpinning rational design and scale-up of continuous crystallisation platforms, in the context of solid material processing.

We have a strong and diverse core academic team, who also bring strong additional collaborations to the CMAC-SPIRIT effort. The core academic team straddles four institutions, and the disciplines of Chemistry, Chemical Engineering and Pharmaceutical Sciences.

Alastair Florence, University of Strathclyde (alastair.florence@strath.ac.uk)

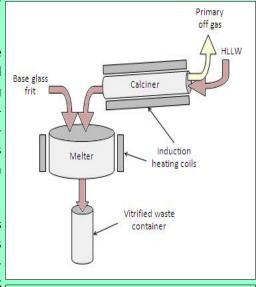
Multivariate Data Fusion for Predictive Modelling and Performance Monitoring

Sellafield Ltd and the National Nuclear Laboratory have collected and collated large amounts of data from various measurement points throughout the nuclear waste treatment plant at Sellafield, most specifically from the vitrification of high-level liquid wastes. These readings include pressures and differentials, glass pour rates, temperatures, and power consumptions from throughout the waste vitrification plant (WVP) and the inactive vitrification test rig (VTR), with some readings taken as often as every half a second over the

course of several years. This vast collection of data provides a repository of historical process information.

The goal of this work is to correctly and appropriately utilise these data, and through the application of data fusion and multivariate analyses, provide higher process understanding and ultimately real-time identification of problems and process deviations. To this end, two process issues were highlighted for improvement; reducing variability in the mass balance of the vitrification process, and optimising operation of the primary off gas system.

The data was mined first hand upon visiting the plant, thus allowing collection of appropriate data for initial work. This initial work included extensive data organisation, pretreatment and algorithm creation, followed by benchmark analysis consisting of "traditional" modelling methods



Schematic of the WVP and VTR

such as principal components analysis and partial least squares. Unfortunately, yet not unexpectedly, these benchmark analyses did not yield information of any great significance, indicating a desire for a more sophisticated method of information extraction and modelling.

More novel methods such as multi-sensor data/information fusion (MSDF or MSIF) and other dynamic methods are currently being investigated, and their feasibility for these datasets evaluated. Ultimately, a methodology will be developed to allow predictive models to be created to identify the causes of the specified problem areas, with the aim of facilitating process understanding and optimisation, whilst improving on the results obtainable via more traditional established methods.

The basic premise of MSDF is the fusion of several sources of information/sensors/measurements to build understanding of a process or object. It can be thought of analogously as how humans fuse together sight, taste, smell, hearing and touch to process information and make decisions. Many applications of MSDF currently reside in the field of military and defence, weather prediction and monitoring, and in robotics. Applications in industry are still not fully investigated and applied.

Currently, I am studying MSDF frameworks that use methods of Bayesian inference, and ones that use an artificial neural network approach. This involves familiarising myself with the Bayesian interface and theory, which in itself is an intriguing topic. I will then go on to learn how this connects to the MSDF framework. After this, implementation of the method on the existing datasets will be attempted.

Stephanie Turnbull,

CPACT, University of Strathclyde