CENTRE FOR PROCESS ANALYTICS AND CONTROL TECHNOLOGIES

CPACT NEWSLETTER — April 2009

5-7 May 2009
The Hilton Hotel, Glasgow

There is still time to register for the APACT 09 conference, please visit: www.apact.co.uk for more details or contact: natalie@cpact.com

CPACT Research Day
Tuesday 10th March 2009

We had an excellent CPACT Research Day at the University of Strathclyde with very interesting presentations and poster session.

For those who were unable to attend this event, please note that the presentations are now available on the 'members only' section of the CPACT website, to view visit:

http://www.strath.ac.uk/Other/cpact/mo/themes.htm

RECOGNITION FOR CPACT IN THE RESEARCH ASSESSMENT EXERCISE

The Centre for Process Analytics and Control Technology (CPACT) in the School of Chemical Engineering and Advanced Materials at Newcastle University was highlighted in the recent Research Assessment Exercise as exemplifying Esteem in terms of contributions external collaboration and impact of the research on quality of life.

CPACT TEAM

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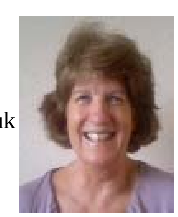

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Near-infrared optical analytical technologies for online/non-invasive characterization of chemical and biological systems

In October 2008 I moved from Newcastle to Strathclyde University to take up a senior lectureship post in the department of chemical engineering. My decision was prompted by the fact my research interests fit well with Strathclyde's strengths in analytical sciences and photonics. I believe that I could build productive partnerships with researchers in Strathclyde who work in these areas in a way that would greatly expand my research activities.

My research whilst at Newcastle focused on an integrated measurement-interpretation methodology where multiple measurements, in conjunction with the radiative transfer equation which describes multiple scattering effects, are used to separate the absorption and scattering effects. The first step in this approach is to invert the measurements using the radiative transfer equation to obtain the bulk absorption and scattering properties. The second step is to extract the individual species information from these bulk properties. This step involves the development of novel methodologies through combination of physics of light propagation and multivariate statistical methods. At Strathclyde, I will continue developing the methodologies using two measurement configurations – integrating sphere set-up and a spatially resolved measurement set-up.

During my stint in Newcastle, the feasibility of an integrated physics-chemometrics approach based on these configurations for extracting chemical information of suspensions has been investigated. This method was used to monitor the optical property changes during a bacterial growth cycle for a simple Bacillus subtilis system. It was shown that the scattering and absorption properties could be consistently extracted from such measurements. Investigations using a simple polystyrene-water system have also shown that the chemical information can be more accurately extracted through this approach than when the current state-of-the-art chemometric methodologies are used. We are now working on extending this approach for extracting chemical information from multi-component samples where the complexity of the sample and particle concentration is at industrially relevant levels. Towards this end, a double integrating sphere and a spatially resolved measurement system which spans the wavelength range of 300-1700nm will be built.

The expertise developed through the research carried out in the past years will be utilised in the execution of a KTP project with Akzo Nobel which is led by Prof. Morris in collaboration with myself. A CASE studentship with Nexia solutions also led by Prof. Morris is due to start in the coming months.

New research topics which take advantage of the expertise available at Strathclyde are also being considered. One such topic which will be in collaboration with Prof. Littlejohn and Dr. Nordon from Chemistry and Dr. Mulholland (Mathematics) is the integration of measurements from complementary spectroscopic techniques to extract maximal information contained in the measurements in a robust manner. In the past decade, the availability of progressively cheap and robust spectroscopy instruments and the increasing importance of online monitoring has made it economically feasible for using multiple instruments to monitor a single process stream in order to obtain multiple chemical (e.g. concentrations) and physical (e.g. particle size distribution) properties i.e. to completely characterize the process stream. In such cases, effective utilisation of overlapping information contained in the different measurements in order to overcome problems encountered in the interpretation of data from individual measurements becomes highly desirable. Several CPACT industrial members have shown interest in this topic and we hope to submit a proposal to the EPSRC by the beginning of summer.

In addition to these research activities, I am looking forward to fully take advantage of the collaboration potential that propelled me to make the move to Strathclyde by developing new research projects with colleagues in SIPBS and Bioengineering.

Suresh Thennadil
Department of Chemical Engineering
University of Strathclyde

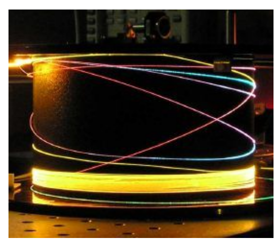
CAVITY RING-DOWN SPECTROSCOPY FOR ULTRA-SENSITIVE CONCENTRATION MEASUREMENTS

Cavity ring-down spectroscopy (CRDS) is a simple technique that can achieve extremely sensitive concentration measurements in chemical processes. It can be capable of detecting substances present at levels even lower than a part-per-billion. Recent developments in light-sources open up opportunities to construct robust instruments for multi-species measurements. This short article gives a brief description of the operating principles of cavity ring-down spectroscopy and provides an example of a novel application of the technique.

The basic technique of absorption spectroscopy relies on the fact that atoms or molecules in a sample will absorb light at certain wavelengths corresponding to a transition to an excited state. Thus the extent of attenuation of a laser beam passing through a sample may be used to determine the concentration of the absorbing species. This seems pretty straightforward but the difficulty is that we often would like to measure concentrations of species present in very low concentrations. This means that only a miniscule fraction of the laser light is absorbed as it passes through the sample and accurate measurement is impossible. A worthwhile analogy is to think of trying to measure the mass of the captain of a ship by first weighing the ship with the captain on board and then weighing it again after he has disembarked. You see the problem.

An obvious way to overcome this difficulty would be to increase the path-length over which the laser absorbs. Often process flows have fixed dimensions but the path-length can be increased by using mirrors to create a multi-pass arrangement where the laser traverses the flow many times. The ultimate extension of this idea is to form a resonant cavity between ultra-high reflectivity mirrors thus permitting effective path lengths in excess of 10 kilometres. This is the basic idea behind cavity ring-down spectroscopy and other related techniques. In the standard configuration of CRDS, we inject a short pulse of light into the cavity. For every round trip a certain amount of light leaks out of the cavity through the end mirror and is detected by a photomultiplier tube. Consequently, intensity of the light inside the cavity is decreasing with time, following an exponential decay. Chemical Engineers may find it useful to think of this exponential decay as representing the 'residence time distribution' of the cavity. The time constant of this decay becomes shorter when an absorbing substance is present in the cavity. From the differences in decay time with and without the absorber (or, alternatively, with the laser wavelength tuned on- and off-resonance) the concentration of the absorbing species can be determined.

An exciting aspect of this involves the proposed use of a novel, high-intensity, broad-band light source known as a supercontinuum or 'white-light laser'. This makes a step forward from previous work since it offers the possibility to perform highly sensitive measurements of multiple species simultaneously rather than being restricted to a single laser for a single species. Preliminary demonstrations of this technique have been performed together with collaborators. Since the light source is robust, fibre-coupled and has low power consumption, it is expected that this new technology should readily find application in industrial process measurements.



A high-temperature nanoparticle synthesis process. The extractive probe shown can be replaced by sensitive cavity-enhanced spectroscopy capable of in situe, non-intrusive measurements

Generation of high-intensity, broad-band, coherent light used for sensitive multispecies detection

Dr Burns recently joined Strathclyde as a lecturer in Chemical Engineering. His research involves the use of laser diagnostic techniques for measurements in reacting flows. A key part of his current research plans involve the use of cavity ring-down spectroscopy and related techniques to detect radical intermediates in nanoparticle synthesis processes in low-pressure flames.

Ian Burns, Chemical and Process Engineering,
University of Strathclyde

THE WATER INDUSTRY RESPONDS TO A CHALLENGE

The latest report from WaterUK[1] concludes that: "***Despite improved efficiency in abstracting, treating and supplying water, population demographics and consumption growth, along with more stringent treatment standards, are driving energy use up.***"

In responding United Utilities decided to look beyond the water sector at how other industries have tackled this problem. They embarked on a collaborative project with Perceptive Engineering Limited and the University of Manchester's Knowledge Transfer Partnership scheme, to investigate the benefits achievable by deploying advanced model predictive control on their wastewater treatment works.

For the majority of the time, the activated sludge plants are run to a dissolved oxygen target setpoint, based on many years of operational experience. Historically when the DO sensors fail (and it is always 'when' not 'if'), sustained quality is maintained by ensuring the plant is sufficiently aerated by over-aerating

Predictive Control begins with a data-derived model of actual plant behaviour. Historical process metrics, representing the broadest possible range of operating conditions, are captured and analysed, to produce a model capable of accurately predicting future process performance. The model predicts the impact that inlet disturbances and variability will have on final quality or capability. It assesses the responsiveness of the current control mechanisms in dealing with those variations. Finally, it calculates – on a minute-to-minute Basis - the optimum series of complex, simultaneous control moves needed to reduce the impact of the disturbances to a minimum; the plant becomes self-monitoring and self-optimising.

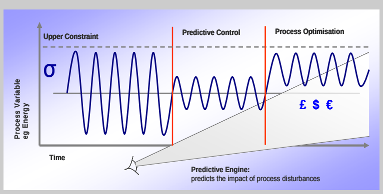


Figure 1.
Predictive control first reduces variability by more effectively managing disturbances, then optimises the process more tightly towards constraint limits.

A process unit controlled this way requires minimal operator intervention to maintain an optimal zone of operation, capable of meeting or exceeding the unit's key performance targets under all conditions.

United Utilities selected their WwTW at Lancaster (100,000 PE) as the proving ground for the technology. The plant was well instrumented, well operated, appears well up UU's 'league table' for efficiency (number 11 out of 65) and was easily accessible. Given the already high performance figures they anticipated no significant improvements and the site trial was purely for 'proof of concept'.

The project brief was simple – demonstrate what is possible from improved control, but under no circumstances compromise the quality of the operation. BOD, COD and ammonia levels were defined as the benchmark. The WwTW consists of three lanes (one closed) each with 5 'pockets' (see figure 1). Typical flow is 30 ML/day, peaking at 90 ML/day. The surface aerators in use represented a further challenge; they are not fitted with variable speed drives so can only be 'on' or 'off' (or 'half speed' in the case of some), controlled either on a fixed timer or via DO level measured in 3 of the 5 corresponding pockets. Would this arrangement be capable of the control resolution required for optimal process operation?

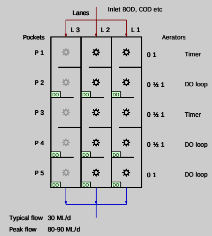


Figure 2.
Schematic of the Activate Sludge Plant at Lancaster. Aerators are either off, on or capable of half-speed. They were controlled by timer or from measured DO.

The project began in late 2007, beginning with a detailed benchmarking and capability assessment. The audit was followed by data collection and analysis, leading to a robust process model *in situ* by early 2008. In-line sensors provided by S::CAN gave real-time measurements of BOD, COD and ammonia in both the inlet and outfall, further minimising the already low risk of transition and adding greatly to the available process knowledge.

At the time of writing, the scheme has been in place for almost a year. Levels of BOD, COD and ammonia have all been maintained well below consent limits, and well below the average required to meet the consent on a 95 percentile basis. Plant operation is both more reliable and more flexible, with substantial headroom for increased load. Compared with their best ever previous performance, United Utilities has calculated **a sustained reduction in energy demand of 26% across the past 11 months**, peaking at almost 50% during the recent Christmas break. This equates to a reduction of about 0.5 kWh per kg BOD[2], or more than 200 Tonnes of CO_2 saved per year.[2]

These results came from a single control system implemented on a single process unit, whose implementation costs will be fully recovered in less than 18 months. The Lancaster site now sits near the top of United Utilities' league table and the project has been put forward for both North West Business and Energy Globe awards.

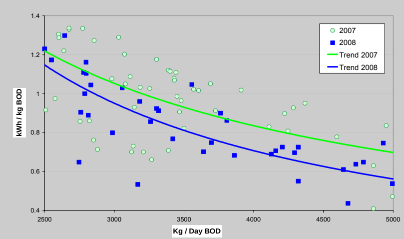


Figure 3: *The new control system has been in place for most of 2008. Compared with energy requirements in 2007 under varying process loads, the new control system has reduced energy variability, and driven down average energy consumption.*

The new control scheme predicts and manages dynamic load changes on the plant, minimising their impact on the operation, while improving the visibility, reliability and efficiency of the process. Plant operation is no longer based on maintaining a dissolved oxygen setpoint; instead, control is focussed on maintaining and improving quality, which is where it always should be.

Simon Mazier
Business Development Manager
Perceptive Engineering

Andrew Wall
Standards & Innovations Manager
United Utilities

Reference:

1 *Sustainable Water: State of the Water Sector Report, Water UK, 17 November 2008.*

2 *Calculations performed by United Utilities Operations team.*