CENTRE FOR PROCESS ANALYTICS AND CONTROL TECHNOLOGIES

CPACT NEWSLETTER June 2013

APACT 13

The APACT conference took place at the Crowne Plaza Hotel in Chester on 24-26th April 2013.

A total of 35 presentations were given over the three days of the conference. There were 3 plenary and 8 keynote talks. 100 delegates attended from countries including Austria, Belgium, Canada, France, Italy, Germany, Norway, Portugal, Spain, Switzerland, The Netherlands, UK and USA. 17 vendor companies exhibited and 10 posters were presented.

Poster prizes were awarded to Nicolau Dehanov, University of Strathclyde (1st prize) for his poster entitled “Spectroscopic monitoring of emulsion polymerization using Kubelka-Munk theory” and Mark Dewar, University of Strathclyde (2nd prize) for his poster entitled “Methods for weighted outlier detection”. Special thanks to Clairet Scientific for sponsoring this prize.

Next year APACT will be taking a break as it’s the Europact 2014 conference which will be held on 6-9th May 2014 in Barcelona. Please put this event firmly in your diaries and further information will be circulated in due course.

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SELLAFIELD LTD—STUDENT RESEARCH PROJECTS WITH NEWCASTLE UNIVERSITY

Carl Steele, Katy Ferguson, Sellafield Ltd

Collaboration with Dr Jie Zhang at Newcastle University has resulted in two Masters projects in association with Sellafield Ltd.

Project 1: James Gray, a final year MEng Chemical Engineering student, has been working on a project for prediction and early warning of melter neck blockages in the Waste Vitrification Plants (WVP), see Figure 1.

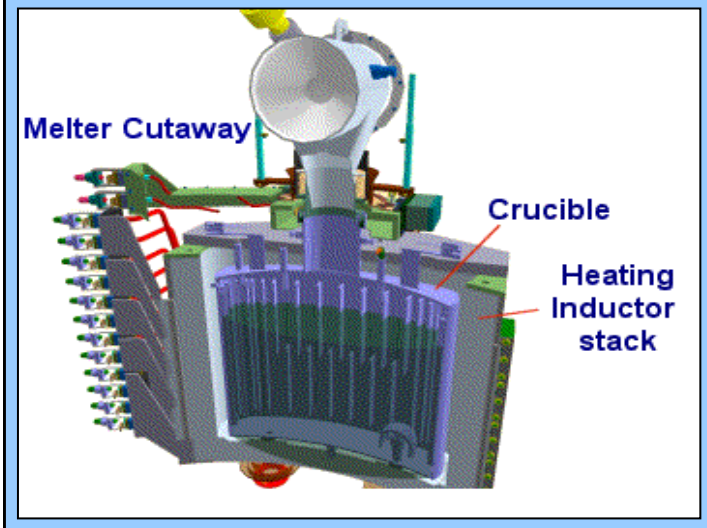

Figure 1: Schematic drawing of WVP melter system

There have been a number of occurrences of melter neck blockages over the last few years, which have caused plant outages requiring recovery in WVP which can take up to two days to complete. An early warning detection could allow intervention to prevent the blockage from occurring or reduce the time required to recover if a blockage had formed.

A melter neck blockage is an accumulation of solidified glass building up over a period of time causing a reduction in the diameter of the melter neck.

When the diameter is reduced to a certain size the flow of calcine and glass are restricted. At this point, an increase in the melter pressure can be observed. The recovery operation is to increase the sparge rate significantly, whilst increasing the melter neck temperature. This process softens and then melts the solidified glass and provides a force to help dislodge the material from the melter neck.

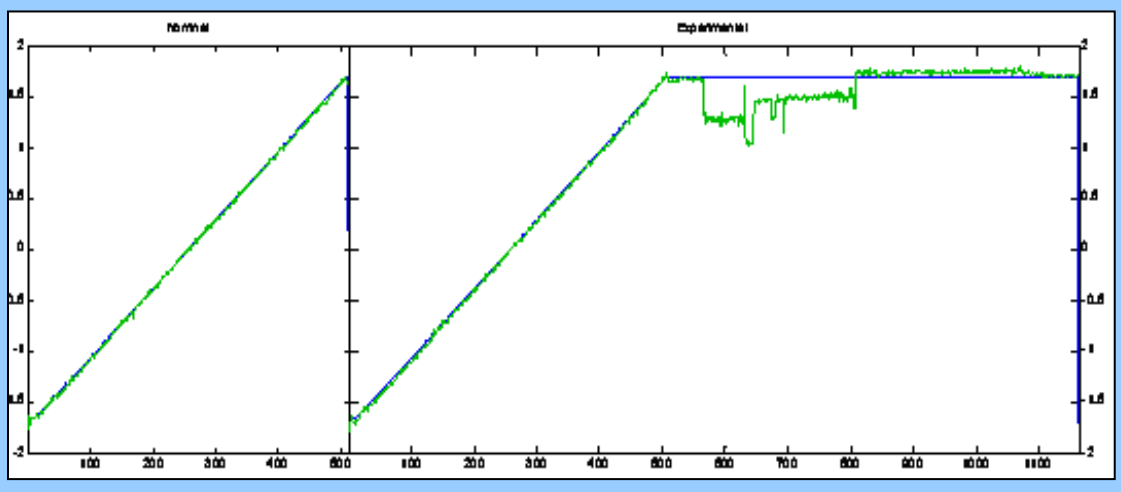

Figure 2: Plot of melter level (y-axis) versus melter mass fed (x-axis)

James completed a study using data collected over a 2½ month period. Data was analysed prior to the event to establish a phase of normal steady-state operation to establish a baseline for comparison.

Principal component analysis was used in this investigation to calculate the relationship between the parameters studied, such as melter level and melter mass feed (Figures 2 and 3).

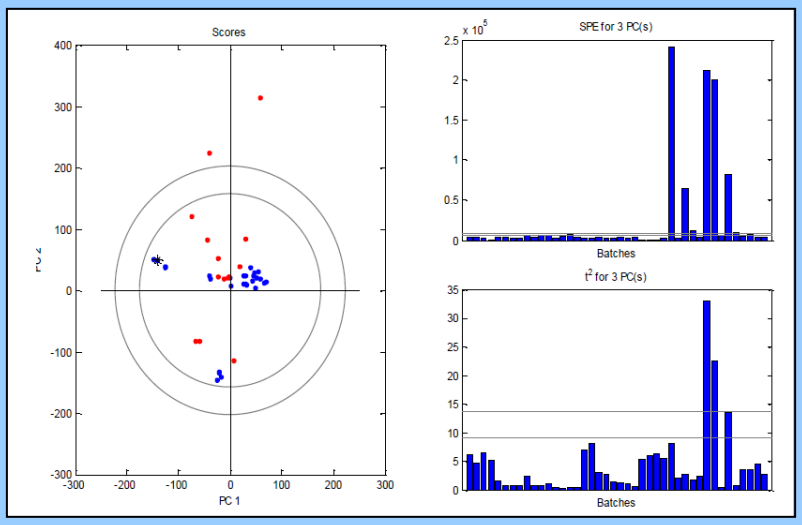

Figure 3: Score plot of batch analysis of the data

James was able to demonstrate that under normal conditions there is a direct correlation between the melter level and total volume flow of highly radioactive liquor to the melter. Under abnormal conditions, as the total volume flow increases the melter level does not increase correspondingly. A significant change in the temperature profile can be observed from measurements taken at the external pour-side apex thermocouple.

Project 2: Damson Kaunga studied the modelling of the chemical durability of highly radioactive waste glass for his MSc project in process analytics.

The use of artificial neural networks (ANN) has been previously applied within WVP to relate molten glass viscosity and feed composition. It was identified that this mathematical technique may also be suitable to relate the elemental leach rate for highly radioactive waste glass.

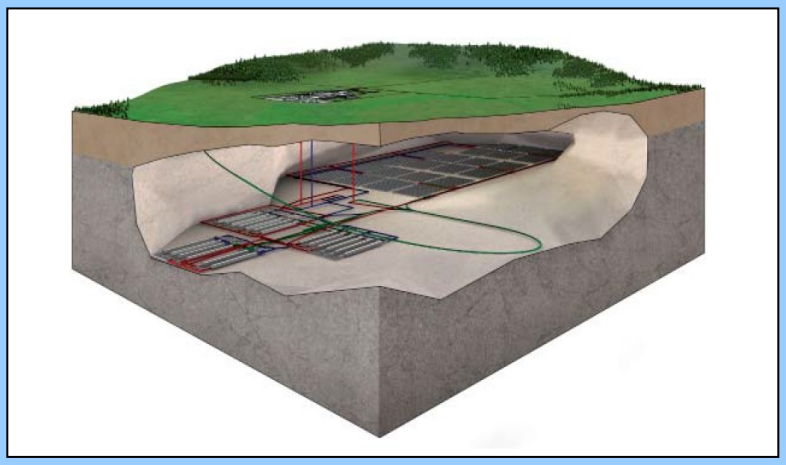

Figure 4: Schematic drawing of the UK Geological Disposal Facility

Modelling of the chemical durability of the highly radioactive waste glass is important for final underground disposal (Figure 4) when it is considered that the material will remain radioactive for several hundreds of thousands of years. Trying to predict the behaviour of the glass is fundamental to understanding how long the radioactivity will be retained in the glass to prevent its release into the geological environment. It would not be possible to measure the durability over a long enough time scale and hence prediction is the only means to estimate how the waste form may behave long term.

Experimental data on non-radioactive glass corrosion, which has been used in this study, was produced by the National Nuclear Laboratory. The results were produced using an American Standard Test Method (ASTM) of durability, the Product Consistency Test (PCT), with variation in experimental conditions, e.g. the ratio of glass surface area to the volume of the leachate solution. A range of different glass compositions was produced and tested.

Four multivariate techniques were used to relate the elemental leach rates of lithium, molybdenum, boron and magnesium to the changing feed composition. It was found that neural network methods produced better predictability than multi-linear regression (MLR) or partial least squares (PLS) with stacked artificial neural networks (SANN[1]) giving the lowest error (see Figures 5 and 6).

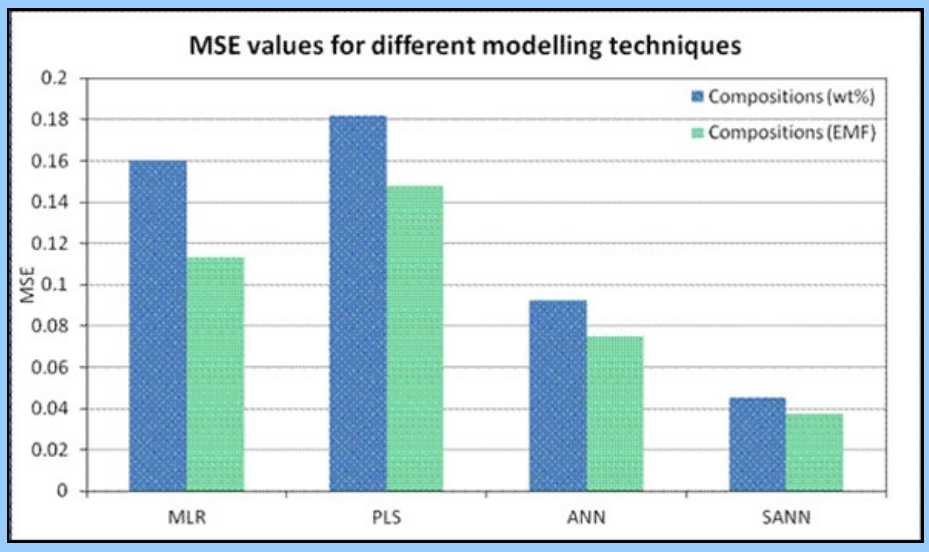

Figure 5: Comparison of the Mean Squared Error for each of the models tested

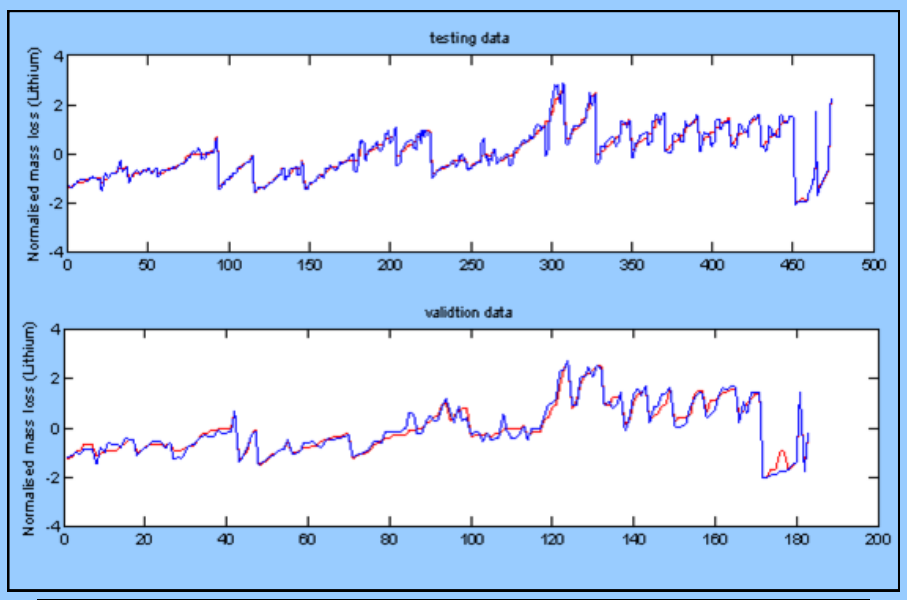

Figure 6: Demonstration of the accuracy for data testing and validation using the Stacked Artificial Neural Network model

The initial findings from this study demonstrated that it would be possible to develop predictability models for glass corrosion. These models could be developed within Sellafield Ltd or form part of a new research study at post graduate level for a PhD funded research project.

[1] J. Zhang, E. Martin, A. Morris, C. Kiparissides, 1997. *Inferential estimation of polymer quality using stacked neural networks*, Computers Chem. Engineering Vol 21, pp 1025-1030

CPACT FEASIBILITY STUDIES

CPACT are now offering 'free' feasibility studies to member companies.

Feasibility studies could be based on a wide range of questions: for example, there might be an interest in assessing a new instrument or instrumental method for process applications, there might be a need to compare different data analysis methods for particular applications, or there may be a need to do some literature evaluation to assess the current status of a developing technology relevant to process analysis or process control. These are just a few examples and it would be up to individual companies to suggest the type of brief study that might be of benefit.

It is important that the scale of the project is kept to a manageable level, especially for an initial investigation. It would be best if feasibility study proposals are:

1. Within the general areas of process analysis, process performance monitoring and chemometrics
2. Focussed on a well-defined topic
3. Capable of being completed within 1-2 months (keep in mind that the re searchers will be doing the work mainly in their spare time e.g. evenings and weekends)
4. Based on the timescale, will cost CPACT no more than £2-3K (including reasonable travel costs to visit the company if necessary)

If members are interested in submitting a feasibility study or would like more information, please contact **Natalie Kerr (natalie.kerr@strath.ac.uk)** for the pro-forma.

DATES FOR YOUR DIARY

PROCESS SPECTROSCOPY COURSE

24-26 September 2013,
Clairet Scientific, Northampton

CPACT RESEARCH DAY

8 October 2013,
University of Strathclyde, Glasgow

CPACT STEERING COMMITTEE MEETING

9 October 2013,
University of Strathclyde, Glasgow

CPACT NEWSLETTER

Do you have an article to contribute to the CPACT newsletter?

If so, we would love to hear from you. Please email your articles to:

natalie.kerr@strath.ac.uk