

Rapid Reaction Analysis workshop at University of Strathclyde, Glasgow on 7-8 September 2011



The first meeting organized by [Rapid Complete Reaction Analysis](#) focus area of the **Dial-a-Molecule** Grand Challenge took place on **7-8 September 2011**. Hosted by the **Department of Pure and Applied Chemistry at University of Strathclyde, Glasgow** the two day meeting brought together 19 delegates from industry and academia. The meeting tackled one of the crucial challenges facing chemistry today: *how can we analyse the reactions much faster, ideally in real-time*. It looked at the technologies currently available and how they can be used for real-time reaction analysis and which developments are required in instrumentation and data analysis methodologies to enable wider use.

The meeting was opened by Prof. Richard Whitby (University of Southampton) who framed the **Dial-a-Molecule** Grand Challenge for the participants as well presenting the expected outcomes of the meeting.

The excellent introduction was followed by a session of plenary talks from industrialists and academics on examples of using reaction analysis (end-users and technology providers). The session started with the talk delivered by Dr. Paul Dallin (Clairet Scientific Ltd.) who presented several examples of reaction monitoring and data analysis. His talk included examples from indirect measurement off gas sampling using MIR spectroscopy, Control of crystal habit using ATR/FT-IR, monitoring fermentation using mass spectrometry as well as microwave-assisted reactions monitored with Raman spectroscopy. He concluded that multidisciplinary teams should include spectroscopists and chemometricians to enable the use of the full armoury of reaction monitoring and data analysis.

There then followed an interesting talk from Dr. Ian Clegg (Pfizer) on Reaction monitoring during development and manufacture of APT. The talk highlighted, among other things, the Pfizer concept of [Lab of the future](#) which includes: interdisciplinary approach, automated lab reactor, rapid analytical tools, automated preparative chromatography and comprehensive informatics. Dr. Ben Taylor (Fibre Photonics Ltd.) presented some of the company products as well as their applications in reaction monitoring (formation of polyurethane prepolymer - which looked at the effect of the catalyst) and biofuel formation.

Prof. Richard Whitby followed with examples of inline analysis of reactions performed in flow systems. Examples included the study of kinetics of ketene formation and the UV monitoring for a photochemical reaction as well as closed loop optimisation for a flow system coupled with a HPLC. The topic of reactions performed in flow was continued by Dr. Christopher Smith (MIT) who presented a case of optimisation in flow in a gas/liquid system and nano-particle synthesis.

Dr. Alison Nordon (University of Strathclyde) introduced the audience to a novel method of process optimisation in micro-reactors based on flow rate manipulation and non-invasive Raman spectrometry. The method provides kinetic information from a single experiment with efficient use of chemicals and equipment delivering comparable kinetic information to the conventional methods.

The introduction to field of microfluidics and their application in reaction analysis was delivered by Prof. Zulfiquir Ali (Teesside University). His excellent presentation provided examples of the wide applications of microfluidics in the transport, mixing and detection of fluids and underlined one of the major advantages of the field: the possibility of delivering instrumentation and a very low cost allowing for its wide spread adoption.

After the lunch Dr. Ian Ashworth (AstraZeneca) presented the use of NMR for reaction monitoring, highlighting some of the advantages and the disadvantages of the technique.

The following two talks focused on the use mass spectrometry for reaction analysis. Dr. Ross Burn (CatSci Ltd.) presented applications of the technique in the development and optimisation of cross-coupling reactions as well as some of the state-of-the-art equipment available (UHPLC-MS, GC-MS, Direct Infusion-MS, etc). Dr. John Langley (University of Southampton) delivered an overview of the MS techniques available nowadays with an emphasis on the wealth of options available to researches. Particular highlights include: Mini11 spectrometer developed at Purdue University, DESI, Direct Analysis in Real Time (DART) Ionisation and the application of TLC-MS using a DART or CAMAG interface.

The series of presentations was closed by the interesting plenary talk given by Prof. Julian Morris (CPACT). His talk, *Rapid Prototyping and Scale-Up in Process Innovation*, focused on moving towards faster scale-up through smart process analytical technologies. He emphasised the fact that Europe provides 32% of the worlds chemicals manufacturing through some 25,000 enterprises of which 98% are SMEs which account for 45% of the sectors 'added value', and 46% of all employees are in SME and asked the question: *How do we ensure that SMEs have access to the latest Rapid Scale-up Technologies?*

The remainder of DAY 1 was dedicated to small group discussions. The discussions focused on identifying the needs and requirements from reaction analysis, barriers to wider use of current technologies and areas where developments are required. Several particular challenges have been identified at the end of the discussions: equipping academia and SME's to use state-of-the-art analytical equipment for reaction monitoring/investigation, automated identification of components in reaction mixtures, enable routine use of sophisticated statistical and modelling, decision tools for deciding which hardware to use for a problem.



The second day of the event was kicked off by a talk given by Dr. Stephen Hillier (Chemistry Innovation). His excellent talk introduced the audience to several funding mechanisms available for the Grand Challenges.

Prof. Richard Whitby followed with a presentation of the main outcomes from the other meetings organized by the [Lab of the Future](#) theme. His presentation was followed by Dr. Alison Nordon who briefly presented the main challenges identified in the previous day and described the expected outcomes from DAY 2.

The presentations were followed, after the coffee break, by small group discussions on the three main challenges identified by participants: equipping academia and SME's to use state-of-the-art analytical equipment for reaction monitoring/investigation, automated identification of components in reaction mixtures, enable routine use of sophisticated statistical and modelling.

The meeting was closed by Prof. Richard Whitby who presented the next steps that will be undertaken by the Real-time reaction analysis focus area and the Lab of the Future theme.

The organising committee would like to thank all the delegates who attended as well the Department of Pure and Applied Chemistry, University of Strathclyde, Glasgow for hosting the meeting and the support provided.