

A paradigm shift in low-field NMR spectroscopy for industrial process monitoring, control, and optimisation: SABRE – Enhanced sensitivity Low field NMR (University of Strathclyde, Dr. Alison Nordon; University of York, Professor Simon Duckett)

The aim of this project is to develop a low cost, low-field nuclear magnetic resonance (NMR) instrument for process monitoring, control and optimisation with the specificity of high-field NMR and enhanced sensitivity. Development of such an instrument requires realisation of the following specific objectives:

1. Development of on-line hyperpolarisation NMR spectroscopy for sensitive detection at low magnetic fields
2. Design of NMR probe sequences employing both radio frequency and magnetic field gradient pulses in conjunction with chemometric procedures for quantitative analysis of mixtures of analytes
3. Demonstration of the instrumentation devised in pilot plant studies with industry
4. Development of on-line hyperpolarisation NMR spectroscopy for sensitive detection in the earth's magnetic field

Successful completion of these activities will enable compositional monitoring not only of bulk components, but also trace 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.

Progress in this project was reported recently at a CPACT Research Day by **Andrew Parrott** from the **University of Strathclyde**. Andrew explained the potential of a bench-top NMR instrument for process analysis when used with hyperpolarisation and signal amplification by reversible exchange (SABRE) with e.g. an iridium complex, to improve the sensitivity of measurement. He also presented the results of a study that used Raman spectrometry to monitor the production of parahydrogen required for hyperpolarisation and its conversion to orthohydrogen, based on the ratio of peaks at 355 and 586 cm^{-1} , which gives the ratio of para:ortho hydrogen. Andrew also described some initial experiments that showed what can be achieved in the on-line monitoring of reactions using the hyperpolarisation procedure.