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Rapid Optimisation of Continuous Flow Processes involving Heterogeneous Nanocatalysts and Reactive Gases

Recently the concept of self-optimising automated reactors incorporating reactor control with feedback algorithms has been utilised to improve the efficiency of chemical reactions and investigate new chemistry. Optimisation has been demonstrated for solution based homogeneous nanoparticle catalysed reactions such as a Heck coupling,[1] a Knoevenagel condensation reaction and the oxidation of benzyl alcohol using the Nelder & Mead Simplex (NMSIM) algorithm[2] with microreactors and on-line HPLC analysis.[3] To date however reactions with gases (either Gas/Liquid or Gas/Liquid/Solid) represent a major class of transformation which still requires significant optimisation, this is additionally complicated by the fact that pressure is an important additional variable which determines the rate of conversion.

This project looks to explore the use of self-optimisation within heterogeneously catalysed processes. To achieve this it will integrate gases into a continuous flow reactor set up (Figure 1) to significantly broaden the scope of reactions which can be studied. Carbon nanostructure (CNS) supported metal nanoparticle catalysts,[4,5] containing well-defined channels and/or pores, will be integrated into fixed bed reactors to explore these novel materials as catalysts to synthesis both exemplar and industrially selected targets.[6] The unique reaction environment within the nanoporous carbon supported catalysts provides enhanced stability and recyclability for precious metal nanoparticles and also leads to increased activity and changes in selectivity. Immobilisation of these materials in a fixed reactor bed will enable; 1) their performance in Gas/Liquid/Solid reactions for selected target synthesis to be assessed, and 2) multistep reactive transformations to be performed, initially focussing on hydrogenation followed by amide bond formation, a common sequence of reactions.

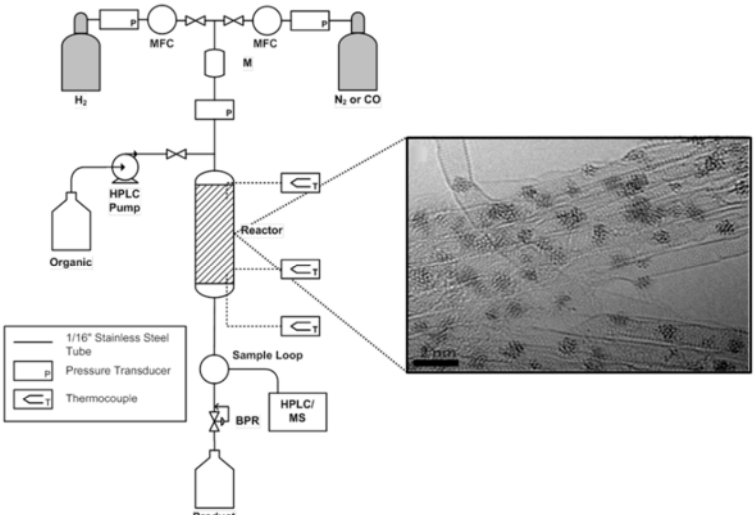

Figure 1. Schematic of a continuous self-optimising Gas/Liquid/Solid reaction system in which carbon nanostructure supported metal nanoparticles catalysts are immobilised in the fixed bed reactor system.

Different projects are available in this area, for example in: (i) fabrication and structural characterisation of novel metallic, bimetallic and mixed metal oxide catalysts supported in CNS; (ii) automated reactor design including the incorporation of mass flow control into continuous flow reactors, and; (iii) industrially led target based reaction optimisation using packed-bed continuous flow reactors. Project work will involve *solid state catalyst fabrication*; *structural characterisation of catalyst materials* including transmission electron microscopy, powder X-ray diffraction, X-ray spectroscopies including XANES and EXAFS and other solid state techniques; automated reactor design and construction; and *synthetic organic chemistry* including flow chemistry.

References

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