Centre for Sustainable & Circular Technologies

Centre for Sustainable and Circular Technologies; University of Bath

Project Title:	Understanding hydrocarbon behaviour in realistic zeolite cracking catalysts using neutron scattering and molecular modelling
Lead Supervisor and co-supervisors:	Dr Alexander O'Malley
Industrial Partner:	Dr Jeff Armstrong from ISIS Neutron and Muon Science

Project Summary

The project will combine neutron scattering and molecular modelling techniques to study the dynamical behaviour of hydrocarbons in acidic zeolite catalysts. Candidates will have a unique opportunity to perform experiments using world class national facilities, alongside complementary modelling to gain insight into one of the most important chemical processes.

Neutron scattering and molecular modelling is a uniquely powerful combination for studying the behaviour of relevant hydrocarbon species confined in the zeolite pores. In particular, quasielastic neutron scattering (QENS) combined with molecular dynamics simulations can probe the diffusion of molecules throughout the zeolite framework, and vibrational spectroscopy combined with quantum mechanical calculations can probe important interactions at the catalyst active site. An important step in studying these systems is to understand the effects of the catalyst regeneration process which causes significant defects due to framework damage, the presence of other FCC species (often bulky molecules which hinder diffusion) and the effect of coke deposits leading to pore blockage/catalyst deactivation.

Candidates would study these effects on the nano- and molecular scale hydrocarbon behaviour in zeolite HY catalysts. The student would also make developments in the simulation led data analysis of neutron experiments through enabling the direct reproduction of QENS observables from molecular simulations, and its integration into routine data analysis packages. The student would therefore gain a unique range of skills in catalysis, neutron scattering, molecular modelling and software development.

The project will be based in the UK Catalysis Hub in Harwell, Oxfordshire, where the student can take advantage of the world class catalyst characterisation and testing facilities, and proximity to the ISIS Neutron and Muon Source.

Sustainability issues addressed

Fluid catalytic cracking (FCC) of crude oil fractions to fuels/base chemicals is one of the largest catalytic processes in the world. It is estimated that >2000 metric tons of FCC catalyst are produced per day, based primarily on acidic zeolite HY. Depleting crude oil resources, and rising CO_2 levels, have driven research into increasing the efficiency of the existing process, but also tailoring the process to accommodate new feedstocks such as biomass, or even waste plastics in existing refineries.