Centre for Sustainable & Circular Technologies

UNIVERSITY OF BATH

Centre for Sustainable and Circular Technologies; University of Bath

Project Title:	Aiding the transition from crude oil feedstocks to biomass: probing the behaviour of relevant hydrocarbon species in acidic zeolite cracking catalysts
Lead Supervisor and co-supervisors:	Alexander J O'Malley, ISIS Supervisor: Jeff Armstrong
Industrial Partner:	ISIS Neutron and Muon Source

Project Summary

The demand for sustainable chemicals and fuels has led to significant research into finding alternative feedstocks to replace crude oil in existing petroleum refineries. Particular focus is on the use of biomass components and their derivatives to generate platform chemicals and fuels. Currently, the majority of these come from the catalytic cracking of crude oil, where it is estimated that >2000 metric tons of fluid catalytic cracking (FCC) catalyst are produced per day, based primarily on the acidic zeolite HY. As petroleum refineries are already in place, the use of this infrastructure for the processing of biomass components should require relatively little investment costs compared to developing entirely new processes. [1]

The current catalysts, Brønsted acidic zeolites, should also be able to play a pivotal role in cracking and upgrading the biomass components, however complexities arise from the higher oxygen content of the substrate which, among other issues, would cause differences both in the behaviour of the molecule at the catalyst active site and the diffusion of the molecules through the catalyst micropores. An understanding of the differences in the behaviour of conventional crude oil based hydrocarbons compared to common biomass components will be crucial in tailoring this technology towards the new feedstock.

Techniques based on neutron scattering, in combination with a range of molecular modelling tools, are uniquely powerful for studying the behaviour of biomass and crude oil relevant hydrocarbon species confined in the zeolite pores. The project will combine simulation techniques with methods such as quasielastic neutron scattering (QENS) and neutron vibrational spectroscopy (INS) to study the diffusion and reaction behaviour of biomass derivatives such as furfurals, in comparison with similar sized but less oxygenated crude oil components in acidic zeolite catalysts. Candidates will have a unique opportunity to perform experiments using world-class national facilities, alongside complementary simulation methods to gain insight into a crucial chemical process of the future.

The student would also make developments in the simulation led data analysis of neutron experiments, and 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.

1. E. T. C. Vogt and B. M. Weckhuysen Chem. Soc. Rev., 2015, **44**, 7342-7370 DOI: 10.1039/C5CS00376H
2. J. Antonio Malero et al. Energy Environ. Sci., 2012, **5**, 7393-7420 DOI: 10.1039/C2EE21231E

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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.