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The application of inelastic neutron scattering and quasielastic neutron scattering to investigate the methanol-to-hydrocarbons reaction over a ZSM-5 zeolite catalyst

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Methanol holds an important role in the chemical manufacturing industry. Not only is it an important commodity on its own but, additionally, it can fulfil a role as a chemical vector and/or an energy vector. An example of methanol being actively used as a chemical vector is the methanol-to-hydrocarbon (MTH) reaction over zeolite catalysts. Methanol is readily available as a feedstock via traditional C1 chemistry routes, whilst the MTH reaction provides access to gasoline grade hydrocarbons for use in transportation fuels. The material that makes the MTH reaction work is the zeolite ZSM-5 [1,2]. Its functionality is exceptional, however not all fundamental physico-chemical aspects of that functionality are well understood. Working towards the development of sustainable chemical process operations, this presentation will outline how neutron scattering techniques can be used to provide a fresh perspective on the operational phase of a working MTH catalyst [1-3].

The concept of a 'hydrocarbon pool' (HCP) is commonly used to describe MTH chemistry over ZSM-5, with the dynamical process accounting for the formation of short chain olefins and methylated aromatics [1,2]. Although understood at a contextual level, details of what constitutes the HCP over the lifetime of a catalyst is not so well defined. This includes its variability with respect to different operational conditions such as temperature.

The presentation will describe a two-pronged approach to investigate aspects of HCP formation over a commercial grade ZSM-5 catalyst active for the MTH reaction [2]. In the first instance inelastic neutron scattering (INS) is used to define the form and nature of the HCP. Three regimes are explored: (i) a catalyst conditioning stage, (ii) steady-state operation and (iii) a catalyst deactivation phase. The resulting spectra indicate the complexity of the HCP but, with referral to suitable reference spectra [4], molecular descriptors for the form of the HCP under the various regimes examined are deduced [5]. Secondly, quasielastic neutron scattering measurements on the post-reaction catalyst samples are used to interrogate how the differing degrees of hydrocarbon retention within the zeolite perturb diffusion within the intricate pore network of the ZSM-5 catalyst.

References

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