Contribution ID: **10** Type: **Poster**

Model lignin monomer dynamics in zeolite catalysts with varying structures and compositions

Tuesday, 11 October 2022 18:40 (20 minutes)

Reducing our dependence on crude oil for producing fuels and commodity chemicals is a major challenge of our time. Lignin is an abundant component of lignocellulosic biomass and has significant potential as a renewable feedstock. Zeolite catalysts will be of great importance for lignin upgrading, not least due to their commercial use in the petrochemical industry, where mixed feeds of biomass and crude oil have already been employed. Probing the fundamental behaviour of model lignin monomers, such as the cresol isomers, within microporous zeolite frameworks is crucial for designing and optimizing the catalytic conversion of lignin into products such as gasoline and other precursors for drugs, dyes and polymers.

To probe the rotational and translational diffusion mechanisms of cresols loaded into zeolites, quasielastic neutron scattering (QENS) was applied.

Initially, the diffusion of bulk liquid cresol from 340-390 K was probed, to aid the parameterization of molecular dynamics (MD) simulations. The linear para-isomer exhibited faster rates of both isotropic rotation and translational jump diffusion, in comparison to meta-cresol. Modelled translational self-diffusion coefficients indicated the same trend.

Upon dosing cresols into zeolites, models of isotropic rotation fit closely to the experimental elastic incoherent scattering function (EISF). A greater population of mobile cresol was observed in the larger pores of zeolite HY (7.4 Å in diameter) compared to the pores of HBEA (6.7 Å in diameter).

Inelastic neutron scattering (INS) has also been employed to probe the zeolite acid site to cresol interaction strengths by analysing changes in the vibrational frequencies of the cresol molecules. The diminishing of peaks relating to the hydroxyl bending of the cresol when inside the zeolite indicates its adsorption to acid sites, which is also essential for catalysis.

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Session Classification: Poster session

Track Classification: Contributions