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## Methanol diffusion in H-ZSM-5 zeolite catalysts as a function of loading and Si/Al ratio

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Establishing sustainable catalysts and processes to achieve renewable energy sources and reduce environmental impact is a pressing matter for the development of our society. The monetisation of natural gas and the high demand for light olefins has resulted in the zeolite catalysed methanol-to-hydrocarbons (MTH) process becoming of high industrial interest. The mobility of methanol molecules to the active site can be affected by factors including Si/Al ratio and methanol loading, having a significant impact on catalyst activity/selectivity. QENS is a powerful experimental tool to probe the nanoscale mobility of methanol in zeolite catalysts, especially in combination with molecular dynamics (MD) simulations. Previous studies of methanol dynamics in ZSM-5 at Si/Al = 36 and 135, showed that upon increasing temperature, the methanol behaviour changes from rotational to translational motion. The translational diffusion is characterised by jump diffusion within spheres of radii close to that of a ZSM-5 channel (similarly observed in a sample with Si/Al = 25). Methanol diffusion in H-ZSM-5 was studied using classical MD at 373 - 423 K, using loadings of 3 and 5 molecules per unit cell, in frameworks with Si/Al = 15, 47, 95, 191 and a siliceous system. While the lower loading exhibits higher diffusivity, self-diffusivities increase at both loadings between Si/Al = 15 and 95, after which they are independent of composition. The trend in diffusivity with Si/Al ratio is explained in terms of methanol-acid site interactions, while the trend with loading is explained in terms of methanol-methanol interactions and the resulting methanol structure in the catalyst pores. MD simulations of the systems have been used to reproduce QENS observables (EISF and QENS broadenings) to ensuring the validity of the employed MD model.

**Primary authors:** WOODWARD, Claire-Louise (University of Bath); Dr O'MALLEY, Alexander (University of Bath)

**Presenter:** WOODWARD, Claire-Louise (University of Bath)

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