CPM9 9th International Workshop
Characterization of Porous Materials:
From Ångströms to Millimeters
May 19 - 22, 2024 | Delray Beach, FL-USA

Contribution ID: **97** Contribution code: **Board 11**   Type: **Poster Presentation**

Extruding diffusion constants from your extrudates: PFG-NMR and chromatography

Monday, May 20, 2024 7:10 PM (20 minutes)

The diffusion of molecules within the confines of a materials pores remains a relatively poorly understood research area. This is despite the diffusion process playing critical role in many adsorption phenomena such as adsorbate selectivity and uptake kinetics. As such, in this work a new model for the analysis of diffusion constants, obtained using a chromatographic Zero-Length Column method, is derived and utilised to accurately determine the micro and macropore diffusion of small molecules in zeolites Na-Y and ZSM-5. In addition to bridging the gap between the NMR and ZLC diffusion analysis techniques.

The proposed mathematical model was derived from the system mass balance, and accounted for fluid-phase contributions, which can be significant in liquid systems[1].

Equation found in attachment

Experimental studies of adsorbate desorption from crystals and extrudates of zeolites Na-Y and ZSM-5 were combined with this mathematical model to determine limiting uptake kinetics.

Figure 1 found in attachment

Fig. 1. A) Simulated diffusion curves with increasing fluid-phase hold-up, γ B) Diffusion models fitted to experimental toluene data from zeolite Y C) A comparison of NMR and ZLC diffusion constants.

Diffusion constants were found to increase in extrudate materials, with a larger contribution of macropore diffusion contributing towards the overall diffusion coefficient. This extrudate diffusion was less affected by surface diffusion, resulting in an increased correlation with diffusion constants obtained from Pulsed-Field Gradient NMR when compared to those obtained from more crystalline samples.

References:
1. Sean R. McIntyre, Elwin Hunter-Sellars, Paola A. Sáenz-Cavazos, Anthony R. Houghton, Daryl R. Williams, Novel zero-length column analysis of desorption curves for single cylindrical pellets, Powder Technology, 416, (2023), 118207.

Acknowledgements:
Thank you to the EPRC and Imperial College London Departmental Scholarship

Primary author: MCLNTYRE, Sean (Surface Measurement Systems)

Co-authors: Prof. WILLIAMS, Daryl (Imperial College London); Mrs SÁENZ-CAVAZOS, Paola (Imperial College London); IACOMI, Paul (Surface Measurement Systems)

Presenter: BURNETT, Daniel

Session Classification: Poster Session

Track Classification: Poster Presentations