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Molecules diffusing and relaxing in macro, meso and microporous materials: An NMR approach for studying the behaviour of fluids confined in nanoporous media

Tuesday, 31 May 2022 17:45 (15 minutes)

Transport and dynamics of fluids in nanoporous networks play a significant role in many applications of porous materials, most notably catalysis, separation and adsorption technologies. Yet, direct experimental measurements of such phenomena at a pore-scale/microscopic level is challenging and key parameters such as diffusion or adsorption coefficients are often extrapolated using indirect macroscopic measurements. In this context, nuclear magnetic resonance (NMR) methods offer some key advantages since they are non-invasive, chemically selective and allow generally fast acquisition of the experimental data. Traditional applications of these methods have been in the area of reservoir engineering and oil/water/rock systems.[1]

In recent years, new applications of such methodologies have been extended to systems such as heterogeneous catalysts, membranes for gas separation as well as soft materials. In this work, the latest developments in these areas are presented. In particular, both high-field as well as newly developed low-field bench-top NMR techniques are used to unravel the behaviour of challenging systems such as photocatalysts and heterogeneous organocatalysts for chemical manufacturing, soft materials for drug delivery as well as mixed matrix membranes for gas separation.[2,3,4] In-situ multi-nuclear (^1H , ^{13}C and ^{19}F) NMR spectroscopy, diffusion and relaxation methods able to provide new and exclusive insights into reaction, diffusion and dynamics of fluids at the solid interface within the pores are used to rationalise and optimise the design of such porous materials, with a particular attention to the structure-transport-activity relationship.

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Country

United Kingdom

References

- [1] Quantitative In Situ Enhanced Oil Recovery Monitoring Using Nuclear Magnetic Resonance, J. Mitchell, J. Staniland, R. Chassagne, E. J. Fordham, *Transport in Porous Media*, 94, 683–706 (2012)
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[3] Tailoring pore structure and surface chemistry of microporous Alumina-Carbon Molecular Sieve Membranes (Al-CMSMs) by altering carbonization temperature for optimal gas separation performance: An investigation using low-field NMR relaxation measurements, L. Forster, C. D'Agostino, M. A. Llosa-Tanco, V. Spallina, C. Brencio, F. Gallucci, M. Lindley, S. J. Haigh, D. A. Pacheco-Tanaka, *Chemical Engineering Journal*, 424, 129313 (2021)

[4] Oxidative coupling of aldehydes with alcohol for the synthesis of esters promoted by polystyrene-supported N-Heterocyclic Carbene: Unravelling the solvent effect on the catalyst behavior using NMR relaxation", G. Di Carmine, D. Ragno, A. Massi, C. D'Agostino, *Organic Letters*, 22, 4927-4931 (2020)

Time Block Preference

Time Block A (09:00-12:00 CET)

Participation

In person

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