What is Happening Inside Catalyst Pores?

Lynn F. Gladden
University of Cambridge, Department of Chemical Engineering and Biotechnology
lfg1@cam.ac.uk

NMR spectroscopy is well-established in characterising and studying the behaviour of both homogeneous and heterogeneous catalysts. However, our understanding of the physical and chemical processes occurring inside the pores of a heterogeneous catalyst remains poor, as a result of the lack of experimental techniques which can study a catalyst in its working environment.

This presentation will describe a number of different magnetic resonance methods that have been implemented to give insight into the world of catalysis within the pore space of the catalyst. These measurements are used to aid the design and selection of heterogeneous catalysts for process applications, and to optimise process operating conditions for a particular catalytic conversion. They also offer opportunities for aiding the development of numerical simulation codes of catalyst behaviour. The following examples will be discussed:

**Adsorption:** NMR relaxation time analysis can be used to characterise competitive adsorption processes at the catalyst surface. This approach can be used for both catalyst and solvent selection.

**Diffusion and Mass Transfer:** The importance of how molecules move through the pore space of the catalyst, and between the pores of the catalyst and the external space between catalyst pellets in the working reactor is often poorly understood. NMR measurements of diffusion and molecular exchange will be presented to demonstrate how these properties of a catalyst can be determined *in situ.*

**Phase Behaviour Inside the Pore Space:** Until now, whether chemical species exist in the gas or liquid state inside the pores of a catalyst has been extremely difficult to determine experimentally. Magnetic resonance methods provide the ability to discriminate and characterise the chemical composition of gas and liquid phases within the catalyst under realistic operating conditions. Such data can greatly aid our understanding of catalyst behaviour.