

Technical & Commercial Progress in the Global Catalytic Process Industries

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Catalytic Advances Program (CAP): Insights and Highlights from Technical Reports

Inside: More Innovation and Competition Boost Polyolefin Catalysts...

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Carmine D'Agostino received a BEng and MEng in Chemical Engineering from the University of Naples "Federico II" (Italy). He then worked few years in the Oil & Gas sector as a process engineer before undertaking studies for a PhD in Chemical Engineering at the University of Cambridge (UK). His doctoral research focused on heterogeneous catalytic processes for the production of fine chemicals using bio-renewable feedstocks. He is currently a lecturer and a research fellow at Cambridge, where he works on the development of new methodologies to characterize the behavior of catalytic materials using NMR and other spectroscopic methods, focusing on understanding the physico-chemical behavior of fluids inside heterogeneous catalysts and functionalised porous materials for catalytic applications. Dr. D'Agostino is the author of over 30 peer-reviewed publications and can be reached at cd419@cam.ac.uk.

The Catalyst Review asked Dr. D'Agostino to share insights he has gained in his investigation of catalyst behavior using NMR spectroscopy and microscopy.

Catalysis represents a major application for porous materials area since these materials are either used for their intrinsic catalytic activity or as supports for catalytically active species, such as metal nanoparticles or coordination complexes. The use of porous solids as catalysts has many practical advantages over homogeneous catalytic processes in solutions; such as, higher thermal stability as well as a much easier handling and separation of the catalyst from the reactive mixture. However, unlike homogeneous catalysts, the structure/stoichiometry relation is complex and often undefined, which makes them less selective and more challenging to study and understand.

Traditional approaches for studying heterogeneous catalyst behavior and performance often rely on the measurement of bulk fluid properties to obtain information on reaction kinetics, rate of reaction, and product distribution. While this is a valid approach to study and rationalize catalyst behavior, it does not provide a comprehensive picture of the process. In particular, an understanding of what is actually happening within the pore space of the catalyst, where the reaction is taking place, is missing. For example, for reactions where products and/or by-products remain trapped in the pore space, there is no way to detect their presence by analysis of the bulk fluid surrounding the catalyst particles. Other phenomena are also missing, such as the extent of fluid/solid contacting, mass-transport and adsorption within the porous matrix, as well as concentration gradients between the inter- and intra-particle space of the catalyst particles.

Several *in-situ* techniques are nowadays available, which are able to monitor catalytic processes close to real conditions. In particular, the use of Nuclear Magnetic Resonance (NMR) methods provides an approach that, together with a more traditional catalyst screening, gives a much more comprehensive picture of the catalytic process. NMR methodologies are non-invasive, quantitative and chemically specific, capable of studying a variety of important phenomena involved in catalysis. These phenomena are not limited to kinetics and product distribution, but also aspects such as molecular transport, surface chemistry, and structural properties of the catalyst.

For example, the use of NMR relaxation time analysis has shown potential as a useful tool for the screening of catalyst surfaces and can also be used to understand solvent effects in catalysis. With this technique, it is possible to probe molecular dynamics and multi-component adsorption of species in catalyst pores, with a relatively rapid acquisition time, by looking at surface-induced changes of relaxation properties of NMR active species inside the catalyst pores. Although most of the research in this field has been carried out within academia, the recent introduction of high-quality low-field portable NMR spectrometers represents a significant progress towards implementing this together with other NMR techniques, on a more industrial/commercial level.

Combined with magnetic resonance imaging (MRI), NMR techniques can be used to study catalytic reactors with temporal but also spatial resolutions and look at spatially-resolved reactor performances within the reactor, such as conversion and selectivity, extent of axial dispersion along the reaction length, temperature profiles, and presence of hot spots as well as hydrodynamic conditions within the reactor. For example, in a recent study on operando magnetic resonance of a fixed-bed catalytic reactor for ethene oligomerization over a Ni/SiO₂-Al₂O₃ catalyst, it was shown that the reaction produces higher molecular weight species early in the reaction, which are trapped inside the pore space, and hence cannot be detected by conventional analytical methods, and are thought to cause deactivation of the catalyst.

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