New Frontiers in Reaction and Catalysis Engineering

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This second volume of *Perspectives in Reaction Engineering and Catalysis* illustrates some of the most innovative ideas in the field, presented by leading authorities. Innovation results from looking across borders, working at interfaces between disciplines, and from borrowing new concepts from one field to apply them to another. Thus, a renaissance in reaction engineering and catalysis today is driven by significant progress in materials science and microtechnology, from the application of quantum chemical and statistical mechanical methods, and by the power of advanced visualization and characterization methods, ranging from the nanoscale to the macroscale (seeing is believing!). This group of articles also demonstrates the need to merge fundamental insights with solid engineering principles, to appreciate the constraints of an industrial setting, and for thinking across length and time scales.

Perez-Ramirez and colleagues shed some light (literally) on industrial porous catalysts, giving an elegant overview of the newest microscopic, spectroscopic and tomographic methods to visualize various processes occurring in catalysts over multiple length scales. They show how the insight that is gained could help not only to characterize catalysts and catalytic processes over time, but also to guide the development of new porous catalysts. Such development requires an integrated approach, from the active site to the reactor level.

Linic and collaborators argue that molecular-level, mechanistic understanding is essential in order to move away from the Edisonian approach of testing endless combinations of catalyst compositions. This understanding facilitates bottom-up catalyst design. Their article illustrates this for the case of metal alloy catalysts. Critical molecular descriptors of catalytic performance are identified, typically the binding energy of a critical intermediate, which can be calculated from quantum chemistry, but does not always have to. A simple model based on

electronic structural parameters is computationally cheaper, and helps to screen configurations and to optimize active sites in order to enhance catalytic performance.

Bhan and *Tsapatsis* present an overview of their recent work on micro/mesoporous zeolites, including three-dimensionally ordered mesoporous imprinted zeolites and self-pillared zeolite nanosheets. Such controlled catalyst architectures over multiple scales may reduce or eliminate diffusion limitations. By using adequate probe molecules, different types of acid sites – internal or external to the zeolitic framework – can be distinguished. Their article points out that it is essential to use modelling approaches to quantify potential transport limitations, and their effects on reactivity. Measuring catalytic rates and comparing them to calculations provides direct information on site accessibility and activity.

The advantages of sophisticated catalyst design can be completely lost by undesirable reactor hydrodynamics, such as maldistribution of fluids. *Sundaresan's* article discusses how high-resolution flow imaging and simulation tools, both of which have progressed dramatically over the past two decades, advance our understanding of the multiscale nature of flows in trickle-bed and fluidized-bed reactors. *Sundaresan* argues that, in multiphase flow, energy from the mean flow is transferred to energy associated with small eddies through slip velocity in between phases, and cascades to energy associated with larger eddies via coalescence of the structures – the opposite of the energy cascade in single-phase turbulence. This insight could help to devise methods to influence macroscopic hydrodynamics, and hereby also reactor performance, by disrupting flow structures at the microscale. Some examples are provided.

The use of magnetic resonance (MR) techniques to image flow hydrodynamics and for in situ catalyst characterization is by now well-familiar to chemical reaction engineers. *Gladden* aims, instead, in her article to introduce some of the emerging areas of the application of MR in the CRE field. Specifically, her paper considers two different types of MR measurements that yield information at two quite different length-scales. They include MR relaxometry and diffusometry in order to study molecular adsorption and diffusion processes within heterogeneous catalysts; and the use of micro-imaging and MR flow imaging to critically evaluate closure relationships and boundary conditions in numerical simulations of catalytic reactors. These measurements have become a recent reality by developments in physical reactor environments that can be operated in a MR magnet, combined with advanced signal processing techniques that are making it possible to explore phenomena that were previously inaccessible to study by MR.

Microreactors have received significant attention in recent years because of potential advantages they offer over conventional systems in terms of enhanced heat and mass transfer and safer operation. *Gavriilidis and coworkers* discuss in their paper the use of such reactors to study intrinsic reaction kinetics, often under conditions that have remained previously unexplored with conventional systems. In particular, their article discusses the prospects for advancing catalytic process development via the combined application of microstructured flow reactors with *in-situ* catalyst characterization and mathematical optimization.

Structured reactors, and in particular catalytic monoliths, are discussed by *Moulijn and Kapteijn*. These are made from a variety of materials (ceramics, metals, polymers, carbon), and are today finding broad applications in the environmental field because of their low pressure drops, their dust tolerance, superior performance, and ease of retrofitting. *Moulijn and Kapteijn* view such reactors as an important tool for process intensification, and their paper makes it clear that their potential value goes far beyond environmental catalysis. They

are applied today, for example, to replace slurry reactors because of their convenience of operation and high selectivity. Their ease and flexibility of preparation makes them ideal for use in many diverse applications, ranging from structured internals in moving-bed systems and catalyst bales in catalytic distillation, to fine chemicals and microreactor applications. The fact that the fundamental aspects of catalytic monolith reactor design are rather well understood (thanks to great measure to the valiant efforts of the authors themselves) makes such reactors ideal and ready to use in many more future industrial applications.

Li, *Xu* and colleagues at Synfuels China show how the combination of insights from quantum chemistry and detailed characterisation methods can be translated all the way from the atomic scale to the rational design of an extremely complex industrial process, namely Fischer-Tropsch synthesis of liquid fuels. Their paper demonstrates how plant design for a crucial energy-related challenge is aided by integrating many fundamental advances illustrated by the other authors in this volume, to realise a successful, full-scale demonstration plant.