How can Magnetic Resonance Contribute to our Understanding of Reaction Engineering Processes?

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Highlights

- Advances in magnetic resonance imaging applied to reaction engineering
- *Operando* studies of Fischer-Tropsch catalysis reveal hydrocarbon composition inside catalyst pores in a real reactor environment
- Images of gas flow and turbulent kinetic energy in a packed bed up to Re_p = 6500
- Direct measurement of liquid-solid mass transfer coefficient in packed beds

1. Introduction

The research undertaken at the Magnetic Resonance Research Centre in Cambridge has multiple aims:

- to use the toolbox of magnetic resonance techniques to give insights to the underlying physical and chemical phenomena underpinning chemical engineering processes and hence optimise, for example, catalyst design and reactor operation
- to acquire data which can be used in simulation codes
- to acquire data which can be used to aid the development and validation of simulation codes
- to develop characterisation methods which can be translated, often on low field magnetic resonance hardware, to the R&D laboratory.

Over the past 20 year there have been significant advances in the development and application of magnetic resonance methods to the application of reaction engineering research. This paper will give an overview of magnetic resonance methods and illustrate the different ways in which magnetic resonance methods can be used. These advances will be illustrated through studies of single- and two-phase flows, including gas-solid fluidisation. More recent work addressing *operando* magnetic resonance studies of Fischer-Tropsch catalytic processes, the direct measurement of liquid-solid mass transfer to a catalyst surface, and the imaging of gas flow and turbulent kinetic energy in packed beds up to a particle-based Reynolds number of 6500 will also be presented.

2. Results

Magnetic resonance is one of the few experimental techniques which can measure both chemical and transport information without need for modification of the system under study. The power of magnetic resonance in application to reaction engineering lies in the fact that multiple magnetic resonance measurements can be combined to study different aspects of the system of interest. For example:

- magnetic resonance imaging (MRI) yields images of the internal structure of the system
- chemically-specific measurements are made through use of chemical shift (NMR spectroscopy)
- pulsed field gradient measurements enable measurement of transport processes, and can differentiate coherent (flow) from incoherent (diffusion, dispersion) processes
- nuclear spin relaxation time measurements can be used to investigate adsorption behavior and the phase (e.g., gas or liquid) in which a molecular species exists.

By using these approaches separately and in combination within a single data acquisition it is now possible to implement measurements which answer specific questions about a reaction engineering process.

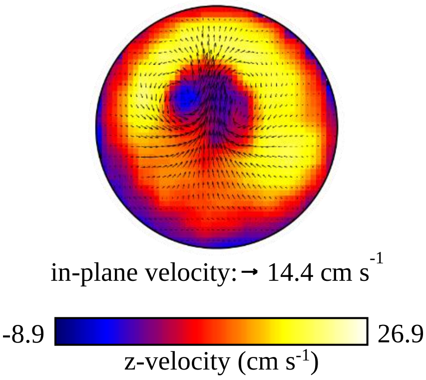

Figure 1. Velocity map immediately under a ‘rising bubble’ bubble of spherically equivalent radius 1.4 mm. Data were acquired at a spatial resolution of 390 μm × 390 μm and the image slice thickness is 1 mm. The field-of-view is 20 mm × 20 mm [1].

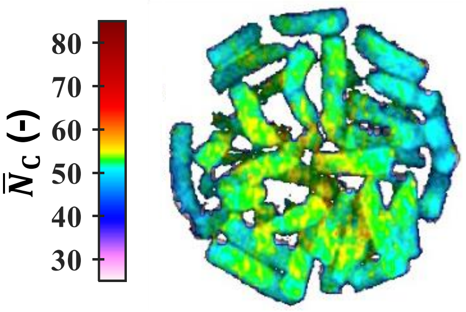

Figure 2. 2D map of average carbon number characterising a hydrocarbon chain within the pores of a ‘working’ Fischer-Tropsch catalyst. The in-plane resolution is 172 μm × 244 μm, and the image slice thickness is 3 mm. The field-of-view is 25 mm × 25 mm [2].

The flexibility in application of magnetic resonance is exemplified by the two examples shown in Figures 1 and 2. Figure 1 highlights the speed at which images of the flow field can be taken using fast imaging experiments combined with data undersampling and compressed sensing image reconstruction strategies [1]. In this experiment, the flow field behaviour which causes oscillations in the orientation of a bubble as it rises in a column was explored. To achieve this image the ‘rising bubble’ was held at a constant axial position through a liquid downflow and the flow field just below the bubble was imaged at a frame rate of 63 frames per second. Figure 2 shows an image of the average carbon chain length in the pores of Ru/TiO_2 catalyst pellets during Fischer-Tropsch catalysis occurring in a packed-bed reactor. The reactor is constructed of non-magnetic silicon nitride, and the reaction is operating at 220 °C and 37 bar. By acquiring a spatially-resolved image of average molecular diffusion coefficient within each image voxel it is possible to obtain the mean carbon number of the hydrocarbon chains within that voxel [3]. Such data give insight as to the real reaction environment within the catalyst pores which in turn informs catalyst design and reactor operating conditions and provides data for input to numerical simulation codes.

References

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Keywords

magnetic resonance; hydrodynamics; reaction engineering; mass transfer