Magnetic resonance methods for studying reactions in trickle bed reactors at operando conditions

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Trickle bed or packed bed reactors are widely used for heterogeneous catalytic process. Improving the performance of the reaction process remains a long-standing challenge because of the difficulty in measuring the actual conditions and concentrations at the scales of both the reactor and catalyst pellet. The motivation for this work is to use magnetic resonance (MR) to measure and understand what is happening inside the pore space of catalyst pellets operating in a trickle bed reactor at realistic conditions (220°C and 36 bar). This work focusses on the application of MR methods to Fischer-Tropsch synthesis which is particularly challenging because of the large number of chemically-similar products that will exist within the reactor. These cannot be separated by 1D ^{1}H spectroscopy due to susceptibility induced line broadening and so other MR methods must be used to obtain information on product distributions. Experiments have been used to spatially map product evolution and the characteristic molecular diffusion coefficients of molecular species within the bed. Figure 1 shows how the spatial distribution of liquid products varies between 2 and 4 days of time on stream. Identification of the composition of those products has been made with diffusion measurements - since all products formed in the Fischer-Tropsch synthesis are hydrocarbons, there is a relationship between the distribution of diffusion coefficients and the distribution of hydrocarbons in the product. From high resolution spatially resolved diffusion measurements, and through suitable calibration, it is possible measure inter and intra pellet product distribution. We show that the product distribution in the pellets is significantly different from that extracted at the outlet of the reactor, which has implications for future reactor design and operation.

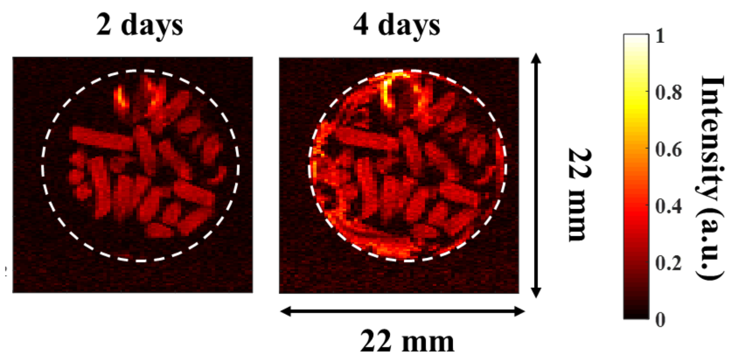

Figure 1. Spatial distribution of products during Fischer-Tropsch synthesis after 2 and 4 days of reaction. Individual catalyst pellets can be seen in the images and the reactor wall is identified by the dashed white line.