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Operando determination of the liquid-solid mass transfer during 1-octene hydrogenation

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In heterogeneous catalysis, the liquid-solid mass transfer process is central to understanding the coupling of mass transport and reaction at the local pellet scale. Measurement of the liquid-solid mass transfer coefficient, k_{LS} , is conventionally made in systems characterised by chemical species and hydrodynamic regimes different from those of the reaction system of interest, or relies on assumed reaction kinetics and the use of a correlation to define k_{LS} . This work reports the first *operando*, direct and non-invasive measurement of k_{LS} . Results are reported for the heterogeneous catalytic hydrogenation of 1-octene occurring in a fixed bed.

The measurements were performed on a fixed bed of 0.3 wt% Pd/Al₂O₃ catalyst pellets under conditions of co-current downflow characterised by liquid and gas Reynolds numbers: $0.2 < Re_L < 0.6$ and $0.1 < Re_G < 0.3$. To achieve this measurement, a novel NMR method was developed in which spatially-resolved ¹³C NMR spectra were analysed using a novel implementation of a partial least square regression [1] method, which enabled discrimination between species in the inter- and intra-pellet space of the reactor. The measurement of chemical composition inside the catalyst pellets (intra-pellet) was made along the length of the reactor with a spatial resolution of 3.1 mm. By combining these measurements with gas chromatography measurements of the reactor feed and exit composition, and direct measurements of catalyst wetting, specific surface area of the reactor and bed voidage obtained from magnetic resonance imaging, the values of k_{LS} were determined to be $0.15 \times 10^{-5} \text{ m s}^{-1} < k_{LS} < 0.25 \times 10^{-5} \text{ m s}^{-1}$. Comparison of these values with correlations reported in the literature showed good agreement with the values predicted from correlations derived from dissolution experiments performed in fixed beds under conditions of similar liquid and gas *Re* to the present study.

The ability to measure local intra-pellet compositions along the length of the reactor also indicated that hydrogenation and isomerisation reactions of 1-octene dominated in the upper and lower regions of the reactor respectively, consistent with the reaction being operated under hydrogen-lean conditions. The NMR data also provided direct evidence of product accumulation inside catalyst pellets due to mass transfer limitation within the system.

This study provides a method by which catalyst pellets and operating conditions can be screened to characterise mass transfer behaviour and aid selection of materials and operating conditions.

Reference:

1. Geladi, P. and B.R. Kowalski, Partial least-squares regression: A tutorial. *Analytica Chimica Acta*, 1986. 185: 1–17.