

From laboratory scale kinetics to industrial reactor simulation: challenges in aromatics hydrogenation

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(Noble) metal catalysts such as Pt, Pd, Ni as well as sulphided NiMo, CoMo and NiW catalysts are known to be highly active for aromatic component hydrogenation [1]. While the former catalysts exhibit the highest turnover frequencies, they are readily poisoned by sulphur components. Hence, hydrotreatment and hydrocracking of heavy oils in the refining industry makes use of the sulphided catalysts to reduce the aromatics content in fuels. Detailed mechanistic investigations of the aromatic hydrogenation kinetics have been performed on the various kinds of catalysts. The major challenge in all this work is that the surface reaction mechanism involves many species that are not directly observable, i.e., that do not desorb from this surface.

While hydrogenation of aromatic components at industrial conditions is typically performed at three-phase conditions, laboratory scale investigation often focuses on vapor phase conditions, especially when an elucidation of the detailed reaction network is aimed at. Having determined the reaction kinetics at vapor phase conditions, they can be implemented in a reactor model that accounts for the presence of a liquid phase, in addition to the gas phase reactants and the solid catalyst [2-4]. Describing the liquid as a non-ideal gas using a cubic equation of state suffices to adequately describe the intrinsic kinetics at liquid phase conditions.

Industrially, hydrotreating and hydrocracking are performed in down flow 'trickle bed reactors', where the gas and the liquid feed are sent concurrently through a fixed bed plug flow reactor. Although the flow pattern in the reactor can be reasonably approximated by the plug flow regime, the observed kinetics in such a trickle bed reactor are quite often affected by transport phenomena [5]. As a result, adequate, industrial reactor simulation models require that these phenomena are quantitatively accounted for. Internal mass transport phenomena and interphase mass and heat transport are identified as the potentially most critical phenomena in trickle bed reactors [6].

In this presentation the determination of a detailed reaction mechanism for aromatics hydrogenation on a Pt catalyst will be discussed first. Subsequently the use of vapor phase determined kinetics in the assessment of liquid phase data will be illustrated. Finally the incorporation of the liquid phase kinetics into an industrial hydrocracking reactor model will be presented and the potential mass transfer effects on the observed industrial reactor behavior will be highlighted.

References

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