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Experimental and theoretical analysis of OCM catalyst deactivation

Aim

Kinetic study of catalyst deactivation upon oxidative coupling of methane over lanthanum oxide-based catalysts

Justification

An ideal catalyst appears unalerted during the reaction, but in reality, the deactivation of catalyst active sites limits the catalyst lifetime and its practical use. That is why understanding the catalyst deactivation mechanism and the rate of deactivation is highly desirable. Within the H2020 ADREM, ERC OPTIMA, and C123 projects, several highly active OCM catalysts were designed at LCT based on lanthanum oxide as the active component. The deactivation rates of these catalysts are not following the same trend, with supported lanthanum oxide being the most stable catalyst. The nature of the catalyst active sites and cause of deactivation are subjects of ongoing studies in our laboratory. Also, several kinetic models have been developed for OCM over mentioned catalysts. However, mathematical expressions of deactivation have not been introduced into the kinetic models yet and will be the aim of this master thesis.

Catalyst deactivation, in general, is a complicated phenomenon considering the presence of several possible deactivation mechanisms with different decay orders and the lack of systemization in this field. In this master thesis, the main information on catalyst deactivation will be available from experimental time-on-stream studies in the fixed bed reactor. Thus, rate expressions can be derived based on the initial catalyst activity. The obtained rate equations will be the basis for developing a deactivation rate formula using both theoretical and experimental time dependant data points. Existing reactor and kinetic models at LCT will be used to develop time-dependent equations and resolve them by minimizing the sum of squares of residues for decay parameters.

This study will provide a fundamental understanding to the OCM catalyst deactivation for the first time. The correlation between active sites of already developed catalysts at LCT and their deactivation rates will provide a novel insight into this field of research that can be used for further stable OCM catalyst design.

Program

1. Literature study: catalyst deactivation mechanisms
2. Literature study: catalyst deactivation theory
3. Kinetic study of the LCT catalysts in fixed bed reactor: time-on-stream performance
4. Developing rate of reaction and including the decay rate formula
5. Identifying the best synthesis approach for designing stable OCM catalyst

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