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Modelling the effect of catalyst deactivation in fluidized bed reactors

Aim

The purpose of this master thesis is to develop a methodology and numerical tool to model the effect of catalyst deactivation, e.g. due to coke formation, in reactors with (ideal and non-ideal) backmixing of the solid phase as e.g. in fluidized bed reactors.

Justification

Catalyst deactivation, i.e., the loss of catalytic activity and/or selectivity over time, is an important problem in industrial catalytic processes. Time scales for deactivation may vary significantly depending on the process. When catalyst deactivation is inevitably fast, such as for methanol-to-olefins (MTO) and fluid catalytic cracking (FCC), fluidized bed reactors are preferred over packed bed reactors since they allow an easy transport of the catalyst pellets to a regeneration unit. The residence time of the catalyst pellets in the reactor, and hence the activity of the catalyst, shows a distribution that depends on the hydrodynamics inside the fluidized bed. This catalyst activity distribution has an important effect on the overall reactor performance and therefore has to be taken into account in fluidized bed reactor models. Nevertheless, many engineering studies of fluidized bed reactors in literature only consider the average catalyst residence time / activity instead of the distribution. Another approach is to use weighted-average reaction rate coefficients, using the residence time distribution as weight function. [1] This is however still an approximation, and possibly, even in the case of ideal solids mixing, only correct in case of linear (first-order) behaviour of the rate expressions.

In this master thesis, an engineering model of a generic fluidized bed reactor will be constructed, using a combination of ideal plug flow of the gas phase and ideal and non-ideal mixing of the solids phase. Several approaches to account for the effect of the catalyst residence time distribution and activity will be implemented and compared with the performance obtained using average characteristics as well as with reactive Computational Fluid Dynamics (CFD) models, for conditions where the above (ideal plug flow and ideal solids mixing) assumptions hold.

Program

- *Literature study on modelling of catalyst deactivation*
- *Implement an engineering model of an "ideal" fluidized bed reactor with generic kinetics*
- *Incorporate the effect of the catalyst residence time and activity distribution*
- *Validation by comparison with more advanced models (e.g., CFD, population balance models)*
- *Application of the developed model to study the effect of coke formation during MTO*

References

1. Bos, A.N.R., P.J.J. Tromp, and H.N. Akse, *Conversion of Methanol to Lower Olefins. Kinetic Modeling, Reactor Simulation, and Selection.* Industrial & Engineering Chemistry Research, 1995. **34**(11): p. 3808-3816.
2. Study of the Coke Distribution in MTO Fluidized Bed Reactor with MP-PIC Approach, January 2019, The Canadian Journal of Chemical Engineering 97(2):500-510. DOI: 10.1002/cjce.23239

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