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Automatic generation of kinetic models for dual active sites mechanisms

Aim

Developing a code for kinetic modelling of catalytic reactions on bifunctional catalysts, i.e., with two different types of catalytic sites.

Justification

The Microkinetic Engine (µKE) is an in-house software tool for the generation of kinetic models[1]. Based on user-specified input information, such as a reaction network, reaction conditions and experimental data, a kinetic model is generated and the corresponding kinetic coefficients can be determined by regression to the data. The output of the tool consists of the model predictions for the dependent variables, as well as the estimated kinetic coefficients including a statistical analysis.

A novel addition to the tool would be the automatic generation of kinetic models for bifunctional catalysts, i.e., with two types of sites. On certain heterogeneous catalysts, multiple different types of catalytic sites are present, which both play an important role in the reaction mechanism. The presence of different types of sites correspondingly requires additional site balances. An example of a reaction catalyzed using a bifunctional catalyst is the hydroisomerization of n-hexane[2]. The reaction can for instance be catalyzed by a Pt-impregnated H-ZSM-5 catalyst. The (de)hydrogenation reactions between the alkanes and the alkenes occurs on the metallic sites, while the isomerization of the alkenes occurs on the acid sites. To test the developed Fortran code, it will be tested on an n-hexane hydroisomerization dataset provided by the Laboratory for Chemical Technology as a case study.

Program

1. Literature study on dual active sites mechanisms in general and n-hexane hydroisomerization in particular
2. Development of a Fortran code for the estimation of kinetic parameters for catalytic reactions on bifunctional catalysts
3. Testing of the code on a n-hexane hydroisomerization dataset as a case study

1. Metaxas, K., et al., *A Microkinetic Vision on High-Throughput Catalyst Formulation and Optimization: Development of an Appropriate Software Tool.* Topics in Catalysis, 2010. **53**(1): p. 64-76.
2. Toch, K.U., J. Thybaut, and G.T.W. Marin, *A systematic methodology for the modeling of intrinsic chemical reaction kinetics: N-Hexane hydroisomerization on a bifunctional zeolite*. 2013, 2013.

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