Kinetic studies of Pd/Al₂O₃-catalyst for three-phase reactions

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1. Introduction

The main goal of the presented studies is to identify another way of process intensification for multi-phase hydrogenation reactions. Therefore the first experimental investigations estimate intrinsic reaction kinetic for a new Pd-catalyst.

The hydrogenation of alpha-methylstyrene (AMS) to cumene in a stirred-tank reactor setup was used as a catalytic model reaction.

2. Methods

The reaction scheme for the Pd-catalysed model reaction is depicted in Figure 1. This catalytic reaction was selected as a model reaction for the estimation of the intrinsic reaction kinetic because of its mildly exothermic characteristic ($\Delta_R H = -109 \, \text{kJ/mol}$ [1]).
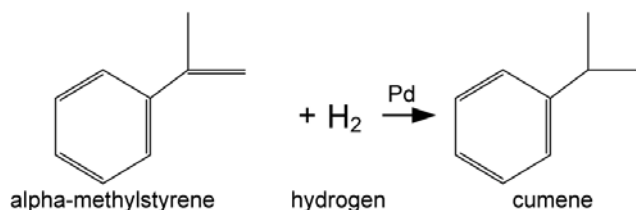

Figure 1. Reaction scheme: Hydrogenation of alpha-methylstyrene [3]

From the literature [2], it is commonly known that there are no transport limitations at temperatures below 320 K for powder catalyst. Besides the individual heat and mass transfer steps in trickle-bed reactors, the intrinsic activity of the new Pd-catalyst is of special importance for the formulation of the reactor model. The estimation of the intrinsic kinetics for the employed catalyst is necessary for further modelling and simulation of dynamic experiments in laboratory trickle-bed reactors.

The used stirred-tank reactor (Parr Instruments Inc., Series 5100, volume 300 ml) is operated in semi-batch mode in which the gas phase is feed continuously to the reactor, which contains the liquid phase (AMS/Cumene). It was proven experimentally that the system can be regarded as isothermal and that transport limitations are absent. Experiments were performed at different temperatures (305 ... 335 K) and hydrogen partial pressures (3 ... 8 bar).

3. Results and discussion

Figure 2 shows typical AMS-conversion-reaction time plots for different reaction temperatures and pressures. The linear and nonlinear dependencies of the AMS-conversion on the temperature are clearly evident.
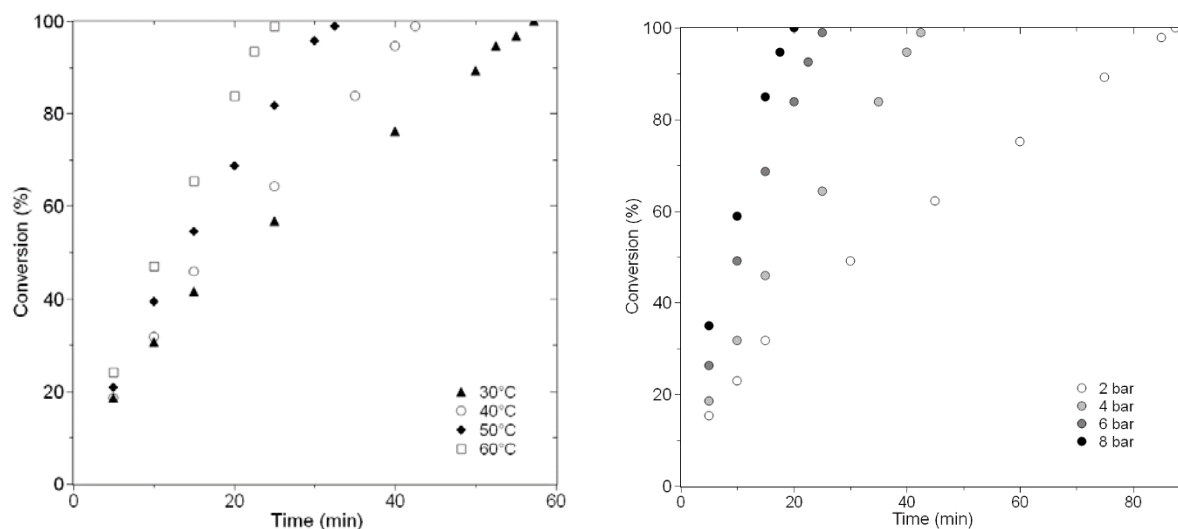

Figure 2. Conversion-time plots for the experiments in the stirred-tank reactor at different reaction temperatures and pressures

The experimental data were applied to estimate the kinetic parameters (e.g. reaction kinetic constant, adsorption constants). Langmuir-Hinshelwood models of the form

$$r = \frac{k\,K_A c_A K_{H_2} c_{H_2}}{(1 + K_A c_A)(1 + K_{H_2} c_{H_2})} \tag{1}$$

or

$$r = \frac{k\,K_A c_A K_{H_2} c_{H_2}}{(1 + K_A c_A)\left(1 + \sqrt{K_{H_2} c_{H_2}}\right)^2} \tag{2}$$

describe the intrinsic activity of the Pd-catalyst. The kinetic parameters (k, K_A, K_{H_2}) for these two reaction rate equations will be calculated by using the experimental data shown in Figure 2.

4. Conclusions

For a new catalyst it is necessary to estimate the specific intrinsic kinetics as one part of the reactor model. Two different reaction rate equations were used to describe the catalytic hydrogenation of alpha-methylstyrene to cumene.

Further experimental data and the estimated kinetic parameters will be presented, discussed and a model recommendation will be given.

References

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