Systematic Validation of Kinetic Models for Heterogeneous Catalysed Gas Phase Reactions

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Minisymposium: Optimum Experimental Design

Abstract: The majority of the chemical reactions used in industrial processes are supported by catalysts. An important application is the waste gas treatment with processes including heterogeneous catalysed gas phase reactions. There they support reactions from undesired to even valuable substances. With the catalyst support higher reaction rates can be reached at lower temperatures what is especially expedient for equilibrium limited exothermic reactions. Here no relevant conversion of educts could be accomplished without catalysts. Huge effort is invested in the development of new catalysts with a higher activity. These new catalysts generally are designed in micro scales. This allows the usage of modern spectroscopic measurement devices which give an insight in the molecular activities. Most of the published work about catalysts is based on the results received at this scale. Anyhow, the catalyst particles used in chemical processes are several scales larger and the encountered mechanisms and kinetic parameter can not be used without further investigations for the reactor layout. Measurements with the commercial catalyst particles are inevitable which means a lot higher experimental effort, because bigger reactors are required.

In this work a systematic approach is presented how to design, built-up and operate a pilot plant for the validation of kinetic models for heterogeneous catalysed gas phase reactions using commercial scale catalyst particles. The core of the plant is the tubular reactor with a diameter of 0.1 m and a length of 1 m. The pilot plant is operated at similar conditions as the industrial scale reactor high gas flow rates are required and with that high performance process units as the heating device and the wet scrubber. High requirements for process automation and safety engineering have to be met. To reduce the number of experiments necessary for reaching a desired model quality the methods of nonlinear experimental design were applied successfully. The results of an exemplary campaign for a sulphuric acid catalyst provided by the BASF SE are presented. It was possible to reach the desired model parameter accuracy with only 8 optimally designed experiments. Anyhow, the operation of a pilot plant under optimal experimental design conditions entails challenges that will be presented here.

This work is supported by the Max-Buchner-Forschungsstiftung.

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