Optimization of methanol synthesis under forced dynamic operation

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Abstract

Methanol is an essential primary chemical in the chemical industry. Further, there is a growing interest in using methanol also for chemical energy storage. Excess electrical wind or solar energy can be converted to hydrogen and react with CO and CO2 from biogas or waste streams to methanol. Suitable kinetic models are required for designing such processes. Established kinetics need to be extended to account for strongly varying input ratios of H2, CO, and CO2 in such applications leading to the need for dynamic process operation. Kinetic models for methanol synthesis accounting for dynamic changes of the catalyst morphology were proposed recently [1].

For the implementation and evaluation of the dynamic operation, a novel reactor concept, incorporating a micro-berty reactor, is established. The configuration allows the modulation of single and multiple input parameters simultaneously, such as partial pressure, total flow-rate, and total pressure. Periodic variation of the inputs results in fluctuating outputs. For the analysis of these changes, an online mass spectrometer (MS) and a micro-gas chromatograph (GC) are implemented for time-resolved concentration profiles, as well as the analysis of collected samples of multiple fluctuation periods.

A set of dynamic experiments is determined by optimal experimental design that improves the parameter sensitivity by solving optimal control problems to identify an optimal parameter set. Additionally, it is analyzed what kind of additional measurement is required for further improvement of the identifiability of the kinetic model [2].

The nonlinear dynamic behavior of the methanol synthesis can be exploited by a forced periodic modulation of different feed streams and total flow-rate (separately of simultaneously) that result in improvements of the time-average output, in comparison to the steady-state process, concerning different objective functions. The nonlinear frequency response (NFR) analysis [3] is used to estimate suitable input variations and the corresponding optimal dynamic parameters (forcing frequency, amplitudes, and phase difference). The NFR method was already applied in various cases [4–6], and it represents promising starting points for rigorous dynamic optimization.

The selection of the objective functions for single- and multi-objective optimization of forced periodic operations is critically discussed.

Keywords: methanol synthesis, dynamic operation, optimization, parameter estimation
P10

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