

Process control strategies and identification of kinetic parameters based on dynamic optimization

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The utilization of existing production networks, still based on petrochemical resources, by integration of renewable feedstocks is a major challenge in process engineering. Long chain olefins have significant potential, e.g. by functionalization in a hydroformylation process to achieve aldehydes which are used as solvents and plasticizers. This is the aim of the Collaborative Research Center Transregio 63 of the DFG. In order to design an optimal process for the hydroformylation of long chain olefins innovative solvent systems are used to recover the catalyst. The underlying thermodynamic fundamentals are investigated and integrated in a comprehensive process design on basis of new methodologies [1]. One decisive part of this work is the identification of the kinetic network and the related reaction rates, which are the basis for the applied optimal reactor design approaches [2].

In this work the hydroformylation process of 1-dodecene in a thermomorphic solvent (TMS) systems consisting of n-decane and N,N-dimethylformamide, respectively, is used to show how optimal control strategies aiming an optimal reactor design can be the basis for appropriate experimental investigations to improve the identifiability of parameters in complex reaction networks (Fig. 1).

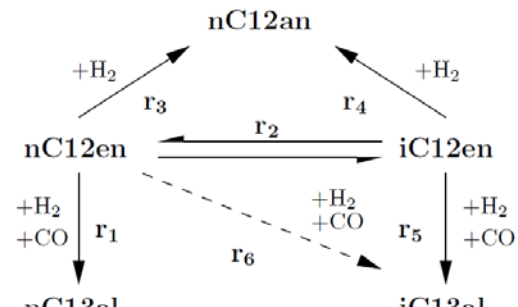


Fig. 1: Reaction network of hydroformylation

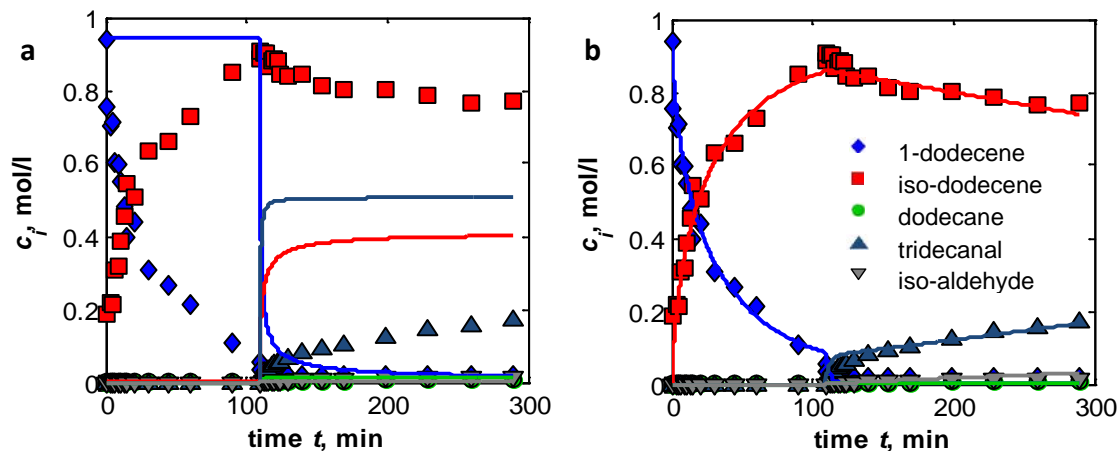


Fig. 2: Experimental (symbols) and modeled (lines) data of a perturbed batch hydroformylation of 1-dodecene based on optimal control calculations. Modeled data without (a) and with (b) re-estimated parameters.

In previous work [3, 4] the network and the corresponding rate parameters have been identified on basis of batch experiments. To improve these kinetics in a wider range of physical conditions optimal control strategies were developed by means of dynamic optimization calculations and validated in further experimental investigations implying batch, semi batch and perturbed batch experiments as illustrated in Fig. 2.

The perturbed batch experiment (Fig. 2) was carried out in two different reaction stages consisting of an isomerization and a subsequent hydroformylation of 1-dodecene to optimize the selectivity towards the linear aldehyde tridecanal. The isomerization of 1-dodecene was started under CO atmosphere at 0.3 MPa and 105°C for 90 min. In the second stage the temperature and the total pressure were raised rapidly to 115°C and 2.3 MPa, respectively, using synthesis gas (CO:H₂ = 1:1) to initialize the hydroformylation of 1-dodecene.

Based on these more sensitive data the improved identification of reaction kinetic parameters maintaining the underlying reaction network was carried out.

This approach leads to an iterative procedure for improvement of kinetic parameter identification, whereby optimal reactor design approaches and parameter identification are combined and performed simultaneously.

Literature:

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