From Data to Miniplant Concepts: An Approach to Accelerate Process Development

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Abstract

In this work, a hierarchical approach to process design and development starting from data to miniplant concepts is presented. It includes the experimental application and practical insights gained from the adaption of a developed optimal model-based design framework for an improved chemical process development. For this purpose, special attention is paid to the explicit modelling of all experimental steps so as to prepare, implement, and analyse experiments in order to have a realistic definition of the numeric design problem and to formally include experimental restrictions and sources of uncertainties in the problem formulation. The proposed framework will be discussed based on the quantification of the reaction kinetics in multi-phase systems using the example of the hydroformylation of long-chain olefins. The developed framework represents a systematic approach to support the development of chemical processes from laboratory experiments to the optimization of complete processes by investigating the design space and quickly screening alternatives.

The case study is concerned with the hydroformylation process of 1-dodecene, a homogeneous catalyzed reaction via transition metals. The main goals for this process focus on an economical catalyst recycling and a high selectivity regarding the linear aldehyde product n-tridecanal. For this purpose, the hydroformylation process in a DMF-decane thermomorphic solvent (TMS) system with a Biphephos-modified rhodium catalyst is investigated. The postulated reaction network was proposed by (Kiedorf et al. 2013) and successfully applied in (Müller et al. 2013).

Literature cited

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