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Abstract

The objective of this work is to propose new methods for assisting and improving the parametrization of models of chemical processes using the measurement obtained during their operation. The Simulated Moving Bed (SMB) process has been chosen as a case study. The SMB is a continuous preparative chromatographic separation process. Its performance depends on several factors which affect the adsorption behavior of the chromatographic system, influenced mainly by the characteristics of the stationary phase of the chromatographic columns, but also by operation conditions such as the temperature. The product quality requirements imposed on the SMB process can be met by choosing conservative operating points, at the expense of the economic performance. More optimal operation conditions can be attained by means of model-based operation strategies, provided that the models represent the characteristics of the chromatographic system adequately. The properties of the solid phase in the columns of a SMB plant differ from column to column and change in time due to factors such as aging or damage. However, the measurements from the process can be exploited for tracking the parameters which reflect the changes in the characteristics of the plant.

The first contribution of this work is an optimization-based method tailored for the estimation of the states and the parameters of the individual columns of the SMB plant. The estimation task is difficult, as typically the measurement information available from the process is scarce. The proposed estimation scheme considers explicitly in its formulation the switchings of the sensors at the product ports. The approach shows a good efficiency in tracking some key adsorption isotherm parameters for each individual column of the plant. Additionally, its computational requirements are acceptable and the effort required for its tuning is reasonable.

The second contribution of this thesis is a new approach for the determination of operation conditions to drive chemical processes to deliver measurements which, if used for parameter estimation, lead to estimate parameters with minimum variance. The operation conditions are determined by designing optimal dynamic experiments online, i.e. during the operation of the process, taking into account the most relevant constraints imposed on the process. It is shown that the solution of optimal dynamic experiment design (ODED) problems is very challenging for systems described by models of large dimensions and with many parameters. This is the case of the SMB process if it is intended to estimate all the parameters of the adsorption isotherms for each individual column. An approach for the reduction of the complexity of the online ODED is proposed. The approach consists of decomposing the original experimental design problem into a series of smaller problems which extend a preexisting experiment. Computational strategies for the application of the scheme online are also proposed, and it is shown that they are critical for the success of the method. The approach drastically improves the tractability of the online design of experiments, as well as the computation times needed to solve them. It is shown that in the SMB case study the online solution of the ODED problems is intractable without the proposed approach. Finally, using the proposed method, a strategy for dealing with model-plant mismatch by means of feedback is suggested. Furthermore, the scheme can be used not only for the SMB process, but for any process described by models based on differential equations.