technische universität
dortmund

Fakultät Bio-und
Chemieingenieurwesen

LS für Systemdynamik
und Prozessführung

Diplomarbeit / Masterarbeit

Optimal Operation of a Continuos Process for the Hydroformylation of Long-Chain Alkenes in a Micellar Solven System

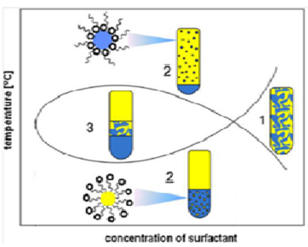
Background and Motivation

The final goal in the operation of any chemical plant is to maximize the profit (optimal economical operation) in presence of disturbances; while different safety, environmental and process constraints have to be satisfied. The issue of optimal economic operation has been traditionally addressed by means of a hierarchical approach: Real-Time Optimization (RTO) [1]. In this technology, an upper layer uses a rigorous static model in order to perform the optimization, while a lower layer performs the regulatory control. As a consequence of mismatch model-plant, the optimal operating point predicted by the model can be different to the actual plant optimum. Among other methodologies proposed, the use of on-line information in the so called *Modifier Adaptation* has proved to be successful in addressing structural mismatch model-plant [2].

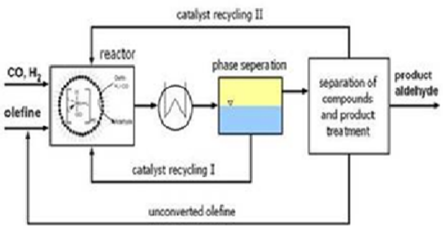
An interesting case of study is the hydroformylation of long chained olefins in a micellar solvent system [3]. In this process, surfactant is contacted with the hydrophilic catalyst and the hydrophobic feed, in order to create a micro-emulsion. The outlet of the reactor is separated downstream in a decanter. The catalyst phase is recycled to the reactor, while the product in the oil-rich phase is sent to further separation and purification stages. The main uncertainties arise from the phase behaviour of the system. The reaction only takes place in a particular region of the phase diagram. Therefore, the estimation of the reactor content is a key element that must be considered in any optimization strategy. There are additional uncertainties in the separation section due to complexity of the phase equilibrium.

Objectives

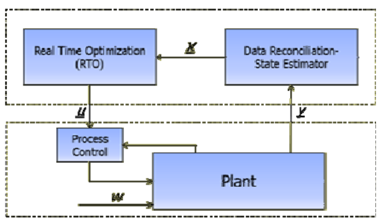
In this thesis a RTO scheme will be developed for the optimal operation of a continuously operated process for the hydroformylation of long chained alkenes in a micellar solvent system. Mismatch model-plant will be addressed by means of Modifier Adaptation. The algorithm will be evaluated theoretically, by means of simulations, considering simplifications to the complex kinetic involved, catalyst deactivation and approximations in the modelling of the phase equilibrium.



Phase Diagram Micellar System



Hydroformylation in Micellar System



Real Time Optimization

Diplomarbeit / Masterarbeit

References

[1] Darby, M. Nikolaou, M. Jones, J. Nicholson, D. (2011) RTO: An overview and assessment of current practice. *Journal of Process Control*, 21: 874-884..

[2] Chachuat, B. Srinivasan, B. and Bonvin, D. (2009) Adaptation strategies for real-time optimization. *Computers and Chemical Engineering*, 33: 1557-1567.

[3] Hamerla, T. Rost, A. Kasaka, Y. Schömacker, R. (2013) Hydroformylation of 1-dodecene with water soluble rhodium catalyst with bidentate ligands in multiphase systems. *ChemCat-Chem 5,* 1854-1862.

Steps

(a) Familiarization with the theoretical background

(b) Getting familiar with the dynamic model available.

(c) Implementation of an estimation strategy

(d) Development and theoretical evaluation of a RTO scheme

Prerequisites

Simulation and programming skills (Matlab and/or C++)

Interest in optimization methods

Start

March 2015

Contact

Reinaldo Hernández. Tel.: 0231 / 755-5135
reinaldo.hernandez@bci.tu-dortmund.de