Dynamic Modelling and Optimization of Intensified Production of Fine Chemicals in Continuous Reactors

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Fine chemicals and pharmaceuticals are still dominantly produced in batch operated stirred-tank reactors. However, continuous production in novel intensified reactors offers much more advantages than a traditional batch process. Intensified reactors, e.g. micro/milli-reactors, oscillatory flow, static mixer etc., radically improve transport properties and thus allow a reaction to approach its intrinsic kinetic limits. This directly relates to improved productivity and selectivity and reduction in energy consumption and waste generation. Yet, there are still open issues connected to operation, design and control of a commercial-scale production of fine chemicals. In this work we are going to analyse design and operational characteristics of intensified reactors by using dynamic optimization and models derived from experimental results for one industrially relevant application.

A commercial surfactant production is selected as a case-study continuous process. The process goals are to have higher production rates (lower reaction times in comparison to the batch), higher surfactant activity and lower reactant and side-product concentrations in the product. The considered reactors are: microreactor, TNO helix and static mixer. The reaction kinetics and the flow properties in these reactors are determined experimentally in bench-scale setups. The validated models are further used for an optimization study. The targets are to offer optimal design and operation of the mentioned continuous reaction systems, by using dynamic optimization. This analysis also examines possibilities for actuation and operation improvement, e.g. optimal feeding of reactants, implementing an optimal temperature profile. The presented results confirm that production of the selected fine chemical in intensified continuous reactors is significantly more efficient than in the batch one and that it can be improved further by advancing actuation and operation.