NEW OPTIMIZATION-BASED APPROACH TO CHEMICAL REACTOR SYNTHESIS – TOWARDS THE FULL INTEGRATION OF REACTOR DESIGN, OPERATION AND CONTROL

Nikola Nikačević[1], **Adrie Huesman**[1], **Paul Van den Hof**[1], **Andrzej Stankiewicz**[2]

[1] Delft Center for Systems and Control, Delft University of Technology, Mekelweg 2, 2628 CD Delft, The Netherlands, n.nikacevic@tudelft.nl
[2] Process & Energy Department, Delft University of Technology, Leeghwaterstraat 44, 2628 CA Delft, The Netherlands

Conceptual chemical reactor design still follows traditional procedure which consists of three sequential stages. In the first stage, operation mode is selected according to the particular reaction and manufacturing demands. The decision is strictly based on heuristic rules, for instance batch operation is preferable for small capacities and multi-products while continuous operation is recommended for bulk production of a single product. In the second stage, reactor is designed according to the reaction kinetics and desirable reactant conversion. Although the reaction volume is calculated using mathematical model, this phase also implies the heuristics, as in most cases predefined reactor type is used for a specific application. In the third phase, a control system is designed for the purpose of maintaining the specified product quality and quantity, as well as process safety. This procedure is well established in the practice; it offers ready-made mathematical models and technical solutions. However, it does not provide optimal reactor design from both economical and environmental perspective.

A new approach to chemical reactor synthesis is going to be presented and illustrated on an example. The concept is based on dynamic optimization which integrates process design, operation and control. The optimization objectives are primarily economical; though it may include controllability and environmental issues. Optimization results should provide optimal operation mode, optimal process design and optimal control policy. This concept promotes the exploitation of process intensification principles and methods for reactor design. It also explores the possibilities for actuation improvement for the optimal control purposes.

Formulation of unique mathematical model which incorporates all revealed issues is not attainable at the present. Therefore, proposed method implies decomposition of a generic problem into two subproblems to be subjected to an optimization. One model assumes distribution of process variables in space and time; while the other assumes variables' distribution only in time, i.e. lumped in space. Consequently, the first model will generate more spatially-oriented solutions, operated often in continuous regime. The second model will result in more timely-oriented solutions, operated more frequently in discontinues or semi-continuous mode. After dynamic optimizations are performed, the target function values will be compared for a selection of the more beneficial solution.

Reactor synthesis methodology is illustrated on the example of parallel liquid phase reactions – esters saponification reactions for a production of sterols. The goal is to have a maximum selectivity and yield of the desired sterol product. The reaction rates are slow and consequently long residence times are needed. The narrow residence time distribution is a general recommendation which will be followed here. The precise temperature control is also an objective. According to the approach two models have been set, one which assumes spatial distribution of concentrations and temperature, and the other with lumped process variables. To approach all of the stated goals, process intensification methods will be implemented. In order to meet requirements for long and narrow residence time, oscillatory baffled reactor (OBR) is an effective option for the spatially-oriented solution. For the case of timely-oriented solution, the fed-batch well mixed reactor (FBR) is chosen. Microwave heating is employed for both OBR and FBR, as it provides volumetric heating which can be easily and rapidly actuated for optimal temperature profiles (in space for OBR and in time for FBR). Actuation is additionally intensified by the optimally controlled feeding of the reactant – spatial feeding in OBR and time-varying feeding in FBR. Optimization target function is based on a profit to be maximized – cost of desired sterol produced minus the approximate investment and energy costs. An open-loop controllability study is performed as well, with another target function which defines the process time response to disturbances, to be minimized. For both systems the optimization provides optimal design (volumes, position of feeding points for OBR) and optimal operation procedures (time variation of feed and input heat). The results have been compared to conventional process performed in batch stir tank reactor with external jacket heating. The results demonstrate significant improvements in selectivity and yield of desired product, which is motivating for further development of presented concept.