A sequential synthesis framework for heat-integrated complex reactor network

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Abstract

Reactor network synthesis is a classical problem in process systems engineering. Main approaches can be classified as heuristic, attainable region and rigorous optimization techniques \cite{1, 2}. However, reactor networks were all optimized under specific reaction path, usually leading to a suboptimal network structure. Furthermore, heat integration should also be taken into consideration for the opinion of energy-saving and emission reduction, which previous researches pay few attention to the effect of heat integration on reactor network synthesis \cite{3}. Therefore, a two-step hierarchical optimization approach for heat integrated complex reactor network is proposed.

In the first step, reaction paths tree and its connection with reactor networks has been discussed. By introducing functional catalysts arrangement, the reaction paths and reactor network could be incorporated in the modified state space superstructure simultaneously. The corresponding mathematical model is formulated as a MINLP problem by coupling kinetics in reaction paths and mass/energy balance equations in reactor networks. A number of alternative reactor networks with specified catalysts arrangement are obtained by the interactive iteration solving method. Then, heat integration of chemical reactors through virtual heat exchangers is employed, allowing the reactor network to be seen as part of the heat exchanger network, leading to a significant decrease in the total energy consumption, while preserving their performance, in terms of chemical transformation. In this work, a case study for p-xylene production is considered to demonstrate the feasibility of the proposed method.