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Optimal reactor design and operation taking catalyst deactivation into account

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Abstract

In this work, a new approach for taking catalyst deactivation into account in the early stage of reactor design is derived and exemplified by the ethylene oxide synthesis as an industrial relevant case study. In this process, the catalyst lifetime is much larger than the residence time of reactants. The operating conditions over the whole catalyst lifetime and the reactor configuration are simultaneously optimized. The objective of the mathematical optimization problem is the overall reactor performance such as the average selectivity over the catalyst lifetime. An optimal detailed design could be derived with advanced temperature control, giving rise to a higher average selectivity and potentially longer catalyst lifetime compared to the reference case.

Keywords: Reactor design, catalyst deactivation, optimization, process intensification, modeling

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