251e Optimization of Periodically Operated Reactor
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Optimal reactor design has focused mainly on steady-state operations. The resulting optimization problems are nonlinear programs whose solution is pursued either through local or global optimization techniques. More recently, periodically operated reactors have caught the attention of reaction engineering researchers because of potentially higher conversions and/or selectivities than traditional devices. Nevertheless, the optimal design of such periodically operated reactors is still underdeveloped.

In our preliminary work, we provided an optimal control formulation for the optimal design of periodically operated reactors, which gave a constrained optimal control problem with periodic boundary conditions. The necessary conditions for optimality were given, strategies for the solution of these equations were outlined, and the method was illustrated on the Van de Vusse process and on a non-isothermal CSTR process.

Application of these methods to the periodically operated reactor problem is outlined. Our work outlines techniques for the solution of the above necessary conditions for optimality. Properties of the associated two-point boundary value problems are discussed and numerical methodologies are outlined for their solution. These methodologies aim at capturing all solutions of the TPBVP and this ensuring global optimality.