79a Optimization Strategies for Simulated Moving Bed and Powerfeed Processes

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Simulated Moving Bed (SMB) chromatography has been gaining more attention since its emergence in the 1960's. Its application areas include sugar, petrochemical, and pharmaceutical separations. In particular, enantiomeric separations have been found to be one of the most effective applications in the past decade.

An SMB system consists of multiple columns connected to each other making a circulation loop. Between every column, there are inlet ports for feed and desorbent streams, as well as outlet ports for extract and raffinate streams. The feed and desorbent are supplied continuously and at the same time extract and raffinate are drawn continuously through the ports. These four inlet/outlet ports are switched simultaneously at a regular interval in the direction of the liquid flow. This system does not reach a steady state but a cyclic steady state (CSS), where the concentration profiles dynamically change, but the profiles of both liquid and solid phase at the beginning of a cycle are identical to those at the end of the cycle.

Determining the design and operating parameters of SMB processes remains a challenging problem. The cyclic dynamics characterized by CSS complicate numerical treatments. In most circumstances of industrial SMB process development, the design and operating parameters are determined by trial-and-error approaches, where dynamic simulations are repeated and the operating parameters are changed manually after every simulation run. In order to avoid this time-consuming process, several approaches are developed that systematically optimize SMB operations. Stochastic optimization approaches as well as Newton-based approaches have been proposed. Currently, development of efficient optimization methods of SMB processes is an active research area.

Many new kinds of SMB operations have been proposed to enhance productivity. Traditional SMB systems keep the liquid velocities constant during a step, and then switch the four inlet/outlet streams at the same time. In PowerFeed systems, however, the velocities become time-variant. Moreover, VARICOL systems perform asynchronous valve switching, where the four inlet/outlet ports are switched independently, not simultaneously. Since the degrees of freedom become significantly larger in these systems, the importance of an efficient and systematic optimization strategy becomes more significant.

In this study we develop two optimization strategies for SMB processes that rely on spatial and temporal discretizations. The first requires only a spatial discretization and applies a sequential dynamic optimization algorithm, while the second requires a temporal and spatial discretization and applies a fully simultaneous optimization approach. In particular, we show that the simultaneous approach is very efficient and well suited for SMB optimization. We begin by describing the SMB model followed by the objective function and CSS constraints. We then describe both optimization strategies. These strategies are compared on the first case study with a linear isotherm, where the advantages of the simultaneous approach are observed. In the second case study, a more challenging system is considered with a nonlinear isotherm. Moreover, in both case studies we show that the simultaneous approach is well-suited for SMB optimization with dynamic feeding strategies.