Optimization of simulated moving bed (SMB) chromatography: a multi-level optimization procedure

Young-il Lim and Sten Bay Jørgensen
Computer-Aided Process Engineering Center (CAPEC)
Department of chemical engineering, Technical University of Denmark (DTU)
2800 Kgs. Lyngby, Denmark

Abstract
This paper presents a multi-level optimization strategy to obtain optimum operating conditions (four flowrates and cycle time) of nonlinear simulated moving bed chromatography. The multi-level optimization procedure (MLOP) approaches systematically from initialization to optimization with two objective functions (productivity and desorbent consumption), employing the standing wave analysis, the true moving bed (TMB) model and the simulated moving bed (SMB) model. The procedure is constructed on a non-worse solution property advancing level by level and its solution does not mean a global optimum. That is, the lower desorbent consumption under the higher productivity is successively obtained on the basis of the SMB model, as the two SMB-model optimizations are repeated using a standard SQP (successive quadratic programming) algorithm. This approach takes advantage of the TMB model and surmounts shortcomings of the TMB model in the general case of nonlinear adsorption isotherm using the SMB model.
The MLOP is evaluated on two nonlinear SMB cases characterized by i) quasi-linear/nonequilibrium and ii) nonlinear/nonequilibrium model. For the two cases, the MLOP yields a satisfactory solution for high productivity and low desorbent consumption within required purities.

Keywords: Simulated moving bed (SMB) chromatography, Simulation, Multi-level optimization procedure (MLOP), Productivity, Desorbent consumption.