288c Efficient Computational Methods to Calculate the Periodic State of Smb Processes

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We demonstrate that the periodic state of the simulated-moving-bed (SMB) process is reproduced by two different single-column chromatographic models:

• One process model in which the part of its outlet stream that is not recovered as product is recycled to the column with a lag of (N-1)*tau time units, where N is the number of columns of the equivalent SMB unit and tau is the switching time;

• Another process model in which the part of its outlet stream that is not recovered as product is recycled to the column with a lead of tau time units, where tau is again the switching time.

Both process models reproduce the periodic state of the equivalent SMB process, because their node balances are obtained from the original SMB node balance by applying the CSS (cyclic steady state) conditions. Although only the first process model is physically realizable, both process models can be implemented numerically and establish a rigorous mathematical framework for developing efficient methods to calculate the periodic state of the SMB process.

The first process model is suitable for approaches based on simulating the dynamics of the single-column operation over a sufficiently large number of cycles, whereas the second process model is appropriate for methodologies based on the complete discretization of both temporal and spatial coordinates of the governing equations for the single column.

In the former case the CSS is established by starting from a judiciously chose initial condition in the single-column model with recycle lag, and simulating the process operation over a sufficiently large number of cycles. The number of cycles normally required to attain the CSS is reduced significantly by employing Shanks transformations to accelerate the convergence. In the latter case the method consists of discretizing the time coordinate for the single-column model over a complete cycle (N*tau time units) and directly imposing the periodic boundary conditions. The resulting system of algebraic equations, obtained after discretization of the spatial coordinate, is solved directly to compute the CSS solution. Both methods provide faster solutions of the periodic state of SMB than traditional approaches.