

79d Theory and Practice of Single-Column Smb Analogs

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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 τ 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 τ time units, where τ 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.

Only the single-column model with recycle lag is physically realizable and we have recently shown how it can be efficiently implemented in practice [1]. Here, we show for the first time a lab-scale version of the unit for the separation of glucose/fructose.

Although only the first process model is physically realizable, both 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 single-column model with recycle lag is suitable for approaches based on simulating the dynamics of the single-column operation over a sufficiently large number of cycles, whereas the model with recycle lead 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 chosen initial condition in the single-column model with recycle lag, and simulating the process operation until CSS is attained. In the latter case the method consists of discretizing the time coordinate for the single-column model over a complete cycle 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.

Finally, we also show that the single-column model with recycle lag is the basis for an experimental setup and procedure to experimentally reproduce the periodic state of the SMB with just one column ($1/N$ th of the amount of stationary phase employed in the equivalent SMB process) and minimum solute and solvent consumptions.

The experimental setup requires four HPLC pumps, which feed the column at variable flow rate with four solutions with different solute concentration: (1) pure solvent, (2) pure solute 1 at feed concentration, (3) pure solute 2 at feed concentration, and (4) normal feed. The four flow rates are continuously manipulated so that the concentration and flow rate of the combined inlet stream mimic those of the ideal single-column chromatographic process.

During the first $(N-1)*\tau$ time units of process operation the solute concentration in the feed stream of the column is pre-computed by process simulation; at later times it is determined from online concentration measurements of the outlet stream taken at $(N-1)*\tau$ time units before. By judiciously

selecting the step within the cycle where the process is started, it is shown that the periodic state can be achieved in just one or two cycles (each overall cycle has a duration of $N \cdot \tau$ time units). Therefore, the solvent and solute consumptions required to experimentally reproduce the periodic state of the SMB process are reduced by a factor of at least 50.

References

J.P.B. Mota, J.M.M. Araújo: *AIChE J.*, Vol. 51, pp. 1641-1653 (2005).