507d Effects of System Parameters and Material Properties on Productivity and Desorbent Consumption in Chiral Smb Separation

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Simulated moving bed (SMB) chromatography is now a practical separation technique for obtaining pure enantiomers because its continuous operation process can achieve both high product purity and high yield. To fully exploit SMB potential, both productivity and desorbent consumption, major contributors of the separation cost, should be considered in the SMB design and optimization. This study systematically examines the effects of system parameters and material properties on productivity and desorbent consumption in chiral SMB separation. The system parameters studied include purity and yield requirements, particle size, column length, total number of columns, column configuration, extra-column dead volume, and feed concentration. The material properties studied include selectivity, saturation capacity, equilibrium adsorption constants (b1 for the low affinity enantiomer and b2 for the high affinity enantiomer), interparticle void fraction, intraparticle void fraction, and mass transfer parameters. The Standing Wave Design considering mass transfer resistances and axial dispersion is used in this study. The Standing Wave Design finds the operating parameters, namely the four zone flow rates and switching time, which give the maximum productivity and the minimum desorbent consumption for a given set of system parameters and material properties. Both linear and nonlinear isotherm systems are studied. The separation of phenylpropanolamine in Chiralpak AD with methanol as the mobile phase is chosen as an example system.

Without any pressure limit, the higher the product purity and yield, the lower the productivity for a fixed set of system parameters and material properties. At a fixed product purity and yield, productivity and desorbent consumption are controlled only by mass transfer efficiency. In this case, small particle size, long column, small extra-column dead volume, or small interparticle void fraction favors high productivity and low desorbent consumption. Long separation zones (the two zones adjacent to the feed port) favor high productivity, whereas long buffer zones (the two zones adjacent to the desorbent port) favor low desorbent consumption. High feed concentration favor high productivity and low desorbent consumption in the linear isotherm region. At very high feed concentrations, however, feed flow rate needs to be reduced to maintain product purity and yield. For this reason, there exists an optimal feed concentration for the maximum productivity.

Under a pressure limit, productivity is smaller than that without any pressure limit. Large particle size, short column, and large interparticle void fraction favor high linear velocity under a pressure limit but they result in low mass transfer efficiency. For this reason, the optimal particle size, column length, and interparticle void fraction for the maximum productivity fall on the boundary between the mass transfer limiting region and the pressure limiting region.

Large saturation capacity, high selectivity, and large intraparticle diffusivity favor high productivity. However, large saturation capacity or high adsorption equilibrium constants increase desorbent consumption. There is an optimal intraparticle void fraction for the maximum productivity because mass transfer efficiency increases but adsorption capacity decreases with increasing intraparticle void fraction. Also, for a given feed concentration, there exists an optimal b2 for the maximum productivity. As b2 increases, the feed velocity increases initially in the linear isotherm region because of the increase in selectivity. However, for very high b2, the feed velocity must decrease because of the nonlinear effects.

The results of this study can guide the selection of SMB system parameters and material properties to increase productivity and to reduce desorbent consumption.