79e Simulated Moving Bed Systems for Center-Cut Separation from Quaternary Mixtures *Jin Seok HUR and Phillip C. Wankat*

Since UOP introduced the first commercial simulated moving bed (SMB) system for hydrocarbon separations, SMB systems have been widely studied, especially for binary separations. Its higher efficiency and lower desorbent usage compared to batch chromatography systems have resulted in a number of commercial applications. On the other hand, SMB applications for multicomponent separations, have been rare. Various configurations of SMB cascades have been proposed and analyzed for multicomponent separations.

If only the most or least retained component in a multicomponent mixture is desired, a single SMB can be used. If the middle (intermediate retained) component is the only desired component, adjusting the adsorbent properties to make it the least or most retained component may be possible. UOP adjusted the adsorbent to make *p*-xylene most retained. Center-cut separations are frequently required in purification steps of bioseparations and adjustment of the adsorbent may not be possible. Examples are insulin purification and sugar separation from biomass hydrolyzate. The center-cut separation may also be required for separation of four stereoisomers.

In previous work (Hur and Wankat, *Ind. Engr Chem. Research, 44*, 1906-1913 (2005)), we introduced a two-zone SMB/chromatography system for complete ternary separations. In this integrated system, A and B are separated by a SMB approach (the switching and remixing with the feed keep the mass transfer zone inside the column) while the B-C separation is chromatographic (the B-C mass transfer zone leaves the system). In this paper we modify the two-zone system, and combine it with a recycled four-zone SMB to separate the intermediate retained component from quaternary mixture (system I). We also develop a recycled cascade with two four-zone SMBs (system II) and compare the systems at the same productivity and D_{total}/F. The quaternary mixture consists of the nucleosides 2'-deoxycytidine (dC), 2'-deoxyguanosine (dG), 2'-deoxythymidine (dT), and 2'-deoxyadenosine (dA) (Paredes et al, *Ind. Engr Chem. Research, 43*, 6157-6167, 2004). Components dC, dG, dT and dA are the least (A), first intermediate (B), second intermediate (C), and most (E) retained components, respectively, and it was assumed that the only desired product is 2'-deoxyguanosine (B).

In the system I, since the BC separation ($_{CB} = 1.30$) is more difficult than the AB and CE separations ($_{BA} = 2.35$, $_{EC} = 2.89$), the quaternary feed is separated into AE and BC mixtures in the two-zone SMB/chromatography and then the BC mixture is separated into B and C products in the four-zone SMB. For purification of only the intermediate retained component (B), some reduction in desorbent use is possible by recycling the unwanted product C product, which includes desorbent, to train 1. Therefore, there are two product streams: ACE mixture from train 1 and B product from train 2.

Several cascades of binary SMBs can be developed for the purification of only the intermediate component (system II). The cascade that separates the feed into ACE and BCE mixtures in train 1, and then the BCE mixture into B and CE products in train 2 proved to be simpler and easier to control compared to other cascades. This cascade employed a recycle stream of undesired dilute CE product back to train 1.

Simulation results showed that the combined cascade, a two-zone SMB/chromatography and a fourzone SMB, can be used for this center-cut separation with reasonable purities and D_{total}/F values, and the capital cost of this system will be smaller than for the recycled cascade with two four-zone SMBs. Although the separation constraints of the system I are more restrictive than those of the system II, the minimum D_{total}/F of the system I is only 3.09, which is much smaller than $(D_{total}/F)_{min} = 9.23$ for the system II. At the minimum $D_{total}/F = 9.23$, the average of purity and recovery of B product in the system I was larger than that of the system II. The system I works best when the CE separation has a large separation factor because the separation is chromatographic.