288a One-Column Analog to Smb for Center-Cut Separation from Quaternary Mixtures

Jin Seok HUR and Phillip C. Wankat

Chromatography is one of the most common methods for chemical analysis and is used for large industrial scale separations. While elution chromatography is an effective method for the analytical scale, countercurrent operation such as a simulated moving bed (SMB) is usually more economical for large scale applications. SMB systems have been widely studied, especially for binary separations, and various configurations of SMB cascades have been proposed for multicomponent separations.

When the middle (intermediate retained) component is the only desired component in a multicomponent mixture, either the adsorbent properties must be adjusted to make it the least or most retained component, or a cascade of SMBs must be used. For example, UOP adjusted the adsorbent to make *p*-xylene most retained to separate *p*-xylene from a mixture of *p*-xylene, *o*-xylene, *m*-xylene and ethylbenzene. For insulin purification and sugar separation from biomass hydrolyzate, a cascade with two SMBs is used.

In previous papers (Hur and Wankat, *Ind. Engr Chem. Research, 44*, 1906-1913, 2005; Hur and Wankat, *Ind. Engr Chem. Research*, 2005 (submitted)), we introduced a two-zone SMB/chromatography system for complete ternary separations and modified the system for obtaining the intermediate component in high purity from a ternary mixture. In this paper we study quaternary mixtures where one of the two intermediate components is desired. A one-column analog system (Abunasser et al, *Ind. Engr Chem. Research, 42*, 5268-5279, 2003) that mimics the two-zone SMB/chromatography system is used for the ternary separation with a middle product consisting of both middle components. This product is sent to a recycled four-zone SMB to produce the desired component as product (system I). A recycled cascade that combines two-zone SMB/chromatography and four-zone SMB systems is studied for comparison (system II). We also develop a recycled cascade with two four-zone SMBs (system III) and compare these systems at the same productivity and desorbent use. 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 for modeling purposes it was assumed that the only desired product is 2'-deoxyguanosine (B).

Since the BC separation ($\square_{CB}$ = 1.30) is more difficult than the AB and CE separations ($\square_{BA}$ = 2.35, $\square_{EC}$ = 2.89), the quaternary feed is separated into AE and BC mixtures in the one-column analog and the two-zone SMB/chromatography in systems I and II, respectively. 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), desorbent use can be reduced significantly by recycling an unwanted product C, which includes desorbent, to train 1.

A cascade of binary SMBs can also be used for the purification of the intermediate component (System III). The cascade that first, separated 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 uses a recycle stream of undesired dilute CE product back to train 1.

Simulation results show that the combined system with the one-column analog and four-zone SMB can be used for center-cut separation from quaternary mixtures 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 for systems I and II are more restrictive than those for system III, the minimum D_{total}/F of systems I and II are only 3.09, which is much smaller than

$(D_{total}/F)_{min}$ = 9.23 for system III. At D_{total}/F = 9.23, the average of purity and recovery of B product in systems I and II was larger than that of system III. Systems I and II work best when the CE separation has a large separation factor.