Journal of Chromatography A, 1418 (2015) 54–76

Contents lists available at ScienceDirect

Journal of Chromatography A

journal homepage: www.elsevier.com/locate/chroma

Speedy standing wave design of size-exclusion simulated moving bed: Solvent consumption and sorbent productivity related to material properties and design parameters

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ARTICLE INFO

Article history:
Received 14 June 2015
Received in revised form 18 August 2015
Accepted 22 August 2015
Available online 29 August 2015

Keywords:
Simulated moving bed
Size-exclusion
Standing wave design
Solvent consumption
Sorbent productivity
Optimization

ABSTRACT

Size-exclusion simulated moving beds (SEC-SMB) have been used for large-scale separations of linear alkanes from branched alkanes. While SEC-SMBs are orders of magnitude more efficient than batch chromatography, they are not widely used. One key barrier is the complexity in design and optimization. A four-zone SEC-SMB for a binary separation has seven material properties and 14 design parameters (two yields, five operating parameters, and seven equipment parameters). Previous optimization studies using numerical methods do not guarantee global optima or explicitly express solvent consumption (D/F) or sorbent productivity (P_R) as functions of the material properties and design parameters.

The standing wave concept is used to develop analytical expressions for D/F and P_R as functions of 14 dimensionless groups, which consist of 21 material and design parameters. The resulting speedy standing wave design (SSWD) solutions are simplified for two limiting cases: diffusion or dispersion controlled. An example of SEC-SMB for insulin purification is used to illustrate how D/F and P_R change with the dimensionless groups. The results show that maximum P_R for both diffusion and dispersion controlled systems is mainly determined by yields, equipment parameters, material properties, and two key dimensionless groups: (1) the ratio of step time to diffusion time and (2) the ratio of diffusion time to pressure-limited convection time. A sharp trade off of D/F and P_R occurs when the yield is greater than 99%. The column configuration for maximum P_R is analytically related to the diffusivity ratio and the selectivity. To achieve maximum sorbent productivity, one should match step time, diffusion time, and pressure-limited convection time for diffusion controlled systems. For dispersion controlled systems, the axial dispersion time should be about 10 times the step time and about 50 times the pressure-limited convection time. Its value can be estimated from given yields, material properties, and column configuration. Among the material properties, selectivity and particle size have the largest impact on D/F and P_R. Particle size and 14 design parameters can be optimized for minimum D/F, maximum P_R, or minimum cost on a laptop computer.

1. Introduction

Size-exclusion chromatography (SEC) has many important applications. Examples include gel permeation chromatography (GPC), for analysis of protein mixtures or obtaining molecular weight distributions of polymers [1,2], and purification of proteins, such as human insulin [3]. However, conventional SEC is a batch process and it is less efficient than simulated moving bed (SMB) for large-scale production.

In SMB, the columns are connected in a circular configuration (loop). Inlet and outlet ports divide the loop into different sections (zones) with different flowrates. A typical 4-zone SMB with two columns per zone (2-2-2-2 configuration) is shown in Fig. 1. The ports are moved periodically to follow the migrating solute bands. The time between port switches is called the switching time, or step time (t_s). The average port velocity (ν) is equal to the column length (L_c) divided by the step time. The separation is achieved by containing the solutes in specific zones. As seen in Fig. 1, the small component (slow solute) is never present in Zone IV while the large component (fast solute) is never present in Zone I. By containing the advancing and trailing concentration waves in their respective zones, pure products can be continuously removed.

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http://dx.doi.org/10.1016/j.chroma.2015.08.042
0021-9673/

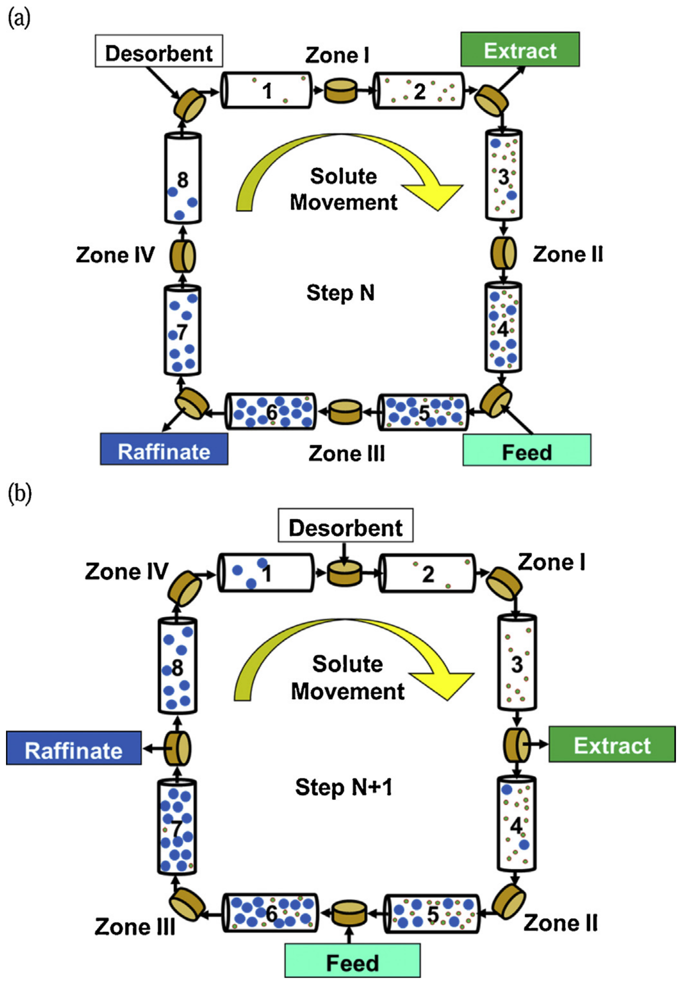

Fig. 1. Diagram of a four-zone SMB. (a) Step N; (b) step $N+1$.

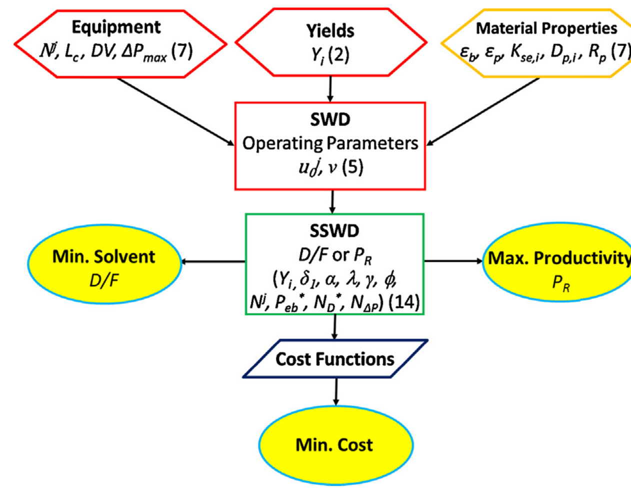

Fig. 2. Design overview.

Size-exclusion simulated moving beds (SEC-SMBs) are more efficient than conventional SEC because only partial separation of solutes in the loop is required to obtain high-purity products with high yield. As a result, a large fraction of the sorbent capacity is utilized and product dilution is reduced. Thus, SMBs consume orders of magnitude less solvent, require an order of magnitude less sorbent, and take up less space than batch operations. Because SMBs are continuous processes, they also require less manpower. These advantages make SMBs economical for large-scale separations.

The SEC-SMB was first introduced by Universal Oil Products (UOP) in 1961 as the Molex process, which separates linear alkanes from branched alkanes [4,5]. SMBs were later developed for adsorptive systems, such as large-scale hydrocarbon purification and high fructose corn syrup production [6]. SMBs for chiral separations have been developed since the 1990s [7]. Lab-scale SEC-SMB have been developed for insulin purification [8,9], separation of myoglobin from bovine serum albumin (BSA) [10], lactose removal from human milk [11], and polyethylene glycol (PEG) fractionation by molecular weight (MW) [12].

Even though SMBs have many advantages, they have not been widely used for large-scale production. SMBs have complex transient and cyclic steady-state phenomena. Equipment for SMBs is often more complex and expensive than batch equipment and SMB experiments are costly and time-consuming. The most important barrier is the complexity of the design and optimization of SEC-SMB. A four-zone SEC-SMB for a binary separation has 21 variables, which include seven material properties and 14 design parameters, Fig. 2. The 14 design parameters include two yield requirements (Y_i), seven equipment parameters, and five operating parameters. The seven material properties are bed void fraction (ε_b), particle porosity (ε_p), two apparent retention factors (δ_i), two intraparticle diffusivities ($D_{p,i}$), and particle size (R_p). The two yield requirements can also be specified as two purities or one yield and one purity. The seven equipment parameters are column length (L_c), dead volume (DV), maximum pressure drop ($\Delta P_{\max}$), and the column configuration (the number of columns in each zone, N^j). The five operating parameters are the four zone velocities (u_0^j) and port velocity (ν). Experimental trial and error with 14 design parameters would be extremely costly. Additionally, the seven material properties, including particle size, can be optimized.

SEC-SMB systems can be optimized for maximum productivity, minimum solvent consumption, or minimum cost. Cost optimizations need to incorporate three main costs: equipment cost; solvent cost, which is related to solvent consumption; and sorbent cost, which is related to sorbent productivity. These costs are controlled by the equipment, material properties, and operating parameters.

The simplest method for designing the five operating parameters is the local equilibrium theory or "triangle" theory. It is widely used and works well for ideal systems (no mass transfer resistance) [13]. However, for non-ideal systems (with mass transfer resistance), this theory only gives the range of possible operating parameters where separation of the components will occur. It does not guarantee purity or yield and it does not give optimum operating parameters for non-ideal systems (most low pressure systems).

The standing wave design (SWD) was first developed by Ma and Wang in 1997 for binary, linear adsorption systems with mass transfer resistances [14]. For fixed material properties, yields, and equipment parameters, the SWD determines the five optimum operating parameters to maximize productivity and minimize solvent consumption. It was extended to multicomponent linear systems [15] and nonlinear systems [16–18]. Pressure limit considerations were incorporated into the SWD [19] by checking that the resulting operating parameters did not violate the pressure constraint.

The SWD method has been incorporated into various optimization routines, based on grid search [9], genetic algorithms [20], simulated annealing [21,22], or combined simulated annealing and genetic algorithm (SAGA) [23]. Optimization variables include particle size (R_p), column length (L_c), column configuration (N^j), and yields (Y_i) [24]. These techniques cannot guarantee global optima and they do not provide an overview of how solvent consumption, sorbent productivity, and separation cost are related to material properties and design parameters.