SMB 공정에서 온도의 영향

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Effects of Feed Temperatures in Thermally Assisted SMB system with Two Feeds

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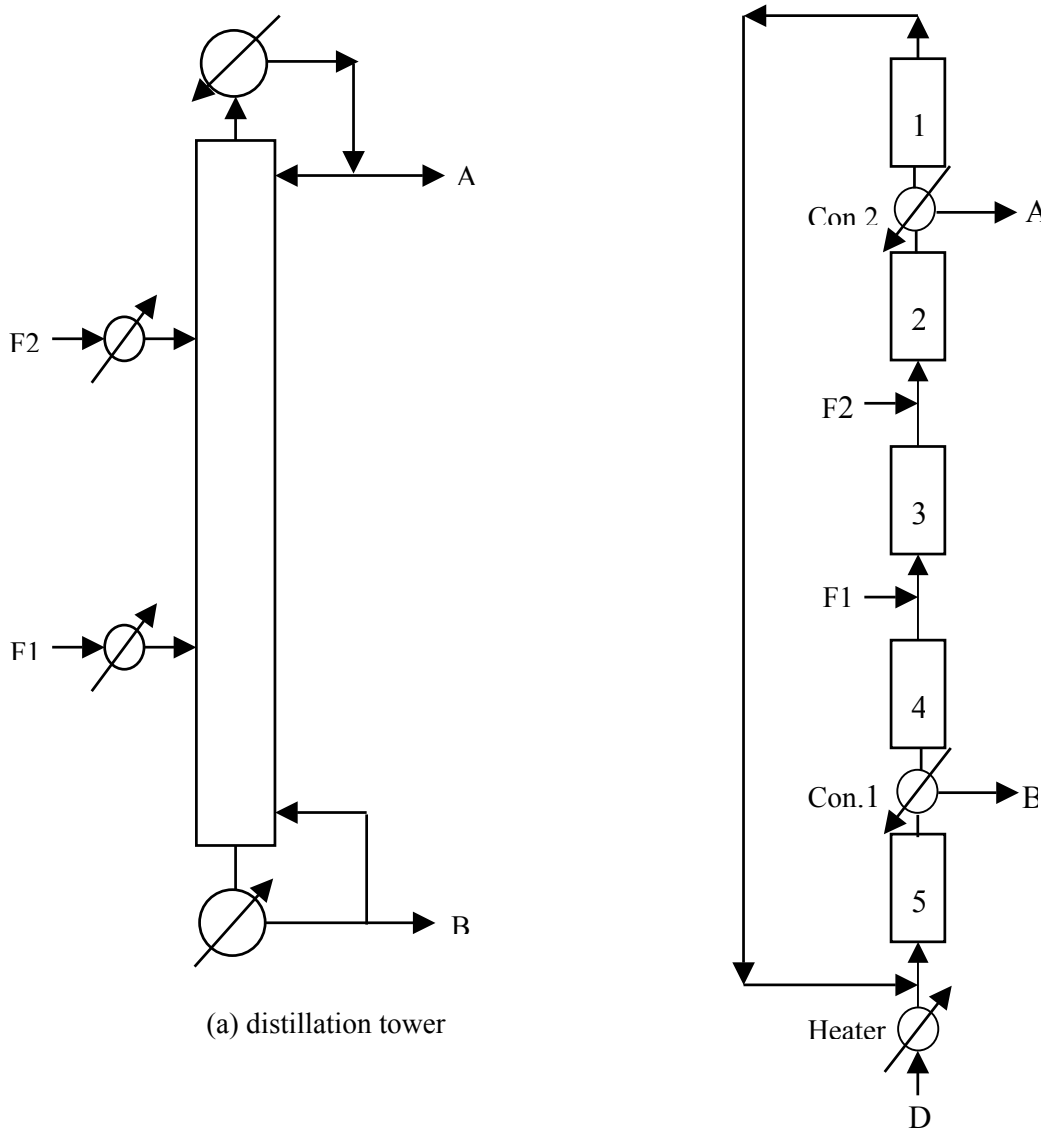
Introduction

Simulated moving bed (SMB) systems are an efficient means of performing large-scale chromatographic separation. Recently, SMB technology has been applied in the food, biotechnology, pharmaceuticals, and fine chemical industries. The isothermal SMB for binary separations has been extensively studied [1, 2].

The use of thermally assisted SMB system is still relatively new and has not been completely examined. Wankat [3] proposed a thermal SMB using the traveling wave mode in which the fluid is heated or cooled. This concept was further studied by Kim et al. [4]. Ruthven and Ching [1] and Migliorini et al. [5] extended the design criteria for linear and nonlinear SMBs, respectively, to study the direct mode where the column is heated or cooled through jackets.

The weak analogy between distillation and SMB systems can be used to develop designs of new SMB systems and qualitatively predict their behavior for the separation of mixtures. Figure 1b shows a single-cascade SMB with two feeds that corresponds to the distillation column shown in Figure 1a. Wankat and Kessler [6] reported that two-enthalpy-feed distillation should be useful in heat-integrated plants and when an ordinary distillation column has a two-phase feed, the use of two-enthalpy feed increased separation or decreased the number of stages, or decreased the reflux ratio.

The objective of this study is to develop a thermally assisted SMB system which improves purities and decreases desorbent usage.



(a) distillation tower

(b) five-zone SMB system

Figure 1. Single distillation tower with two-feeds and corresponding SMB cascade with two-feeds.

Theory

The local equilibrium model for adsorption uses simplified forms of the mass and energy balances to enable analytical calculations. The solid and fluid are assumed to be locally in equilibrium. The mass and energy balances for non-isothermal fixed bed adsorption can be derived by writing differential balances around the solid and fluid phases. If one assumes that radial gradients are negligible, no chemical reactions are taking place, mass transfer is extremely rapid and there is no axial dispersion, the mass balances can be solved for the solute wave velocity.

$$u_s(T) = \frac{v_j}{1+[(1-\varepsilon_e)/\varepsilon_e]\varepsilon_p K_d + [(1-\varepsilon_e)/\varepsilon_e](1-\varepsilon_p)\rho_s \partial q_i/\partial c_i} \quad (1)$$

If the isotherm is linear, $\partial q/\partial c$ is replaced by $K_{eq}(T)$.

Temperature changes force the separation. The velocity of the thermal wave can be obtained from the energy balance. If one assumes the heats of adsorption and mixing are negligible, the column is adiabatic, heat transfer is very rapid, and thermal axial dispersion is negligible, the average velocity of the thermal wave is

$$u_{th} = \frac{v_j}{1+(1-\varepsilon_e)\varepsilon_p/\varepsilon_e + [(1-\varepsilon_e)(1-\varepsilon_p)C_{p,s}\rho_s]/(\varepsilon_e\rho_f C_{p,f})} \quad (2)$$

In a typical liquid system with $T_h > T_F > T_c$, $u_{th} > u_s(T_h) > u_s(T_F) > u_s(T_c)$. The average velocity of port movement is $u_{port} = L/t_{sw}$ .The condition to have A exit in the A product and B in the B product are the same as for an isothermal SMB,

$$u_{A2},\ u_{A3}, u_{A4} \geq u_{port} \geq u_{A1}\ ;\ u_{B5} \geq u_{port} \geq u_{B2},\ u_{B3}, u_{B4} \quad (3\ a, b)$$

In isothermal systems, Eqs. (3) are satisfied by varying the velocities in each zone. In the thermal SMB the solute velocities are also functions of temperature, which adds additional degrees of freedom to satisfy these inequalities.

Local equilibrium calculations and model simulations were done for the separation of a binary mixture of toluene and xylene with silical gel as the adsorbent and n-heptane as the desorbent. Matz and Knaebel [7] reported experimental isotherms and we recalculated the isotherm parameter to satisfy the Arrhenius form, $K_i = A_i e^{B_i/T_j}$. The isotherm parameters for toluene are *A=0.0061* and *B=2175.2695* and for xylene are *A=0.0105* and *B=2115.1052*.

To evaluate the performance of thermally assisted SMB systems with two-feeds at different temperature, the purity index (PI), the average purity of two major components in two products, is defined as

$$Purity\ Index\ (PI) = \frac{Purity\ of\ A\ (\%)\ in\ A\ product\ +\ Purity\ of\ B\ (\%)\ in\ B\ product}{2} \quad (4)$$

Detailed Simulation and Results

Detailed simulations were done using the commercially available chromatography/SMB software package Aspen Chromatography version 12.1. This package is a dynamic simulator that solves the algebraic and partial differential equations for SMB systems. The SMB systems were simulated with two columns per zone. The SMB system was designed for the D/F =1.0 value calculated from the local equilibrium theory in four zone SMB system. Simulation conditions and results are shown in Table 1.

Table 1. Simulation conditions and results. System has two columns per zone and $D/F = 1.0$

Run	Temperature (^oC)					Purity		PI
	Heater	Con.1	F1	F2	Con.2	Raffinate	Extract	
1	298.15	298.15	298.15	298.15	298.15	64.67	69.56	**67.12**
2	323.15	323.15	323.15	323.15	323.15	65.12	70.41	**67.77**
3	353.15	353.15	353.15	353.15	353.15	65.32	70.59	**67.96**
4	323.15	298.15	288.15	293.15	273.15	80.23	85.47	**82.85**
5	353.15	298.15	288.15	293.15	273.15	80.47	85.58	**83.03**
6	353.15	298.15	293.15	288.15	273.15	79.75	86.17	**82.96**

Productivity=0.0105, C_{PS} =920.0(J/Kg/K), C_{Pf} =2243.9(J/Kg/K)

L =100cm, D_c =2.0cm, d_p =0.0335cm, t_{sw} =10.0min, k_A =4.712min^{-1}, k_B =5.5656min^{-1}

F1=F2=16.3759cm^3/min, Raffinate=Extract=Desorbent=32.7518cm^3/min,

Recycle(cm^3/min): Runs 1, 4,5 and 6=102.98, Run 2=113.82, Run 3=135,53

t_{sw} (min): Runs 1,4,5 and 6=10.0, Run 2=6.0, Run 3=3.57

To investigate the temperature effects for a thermally assisted SMB with two-feeds under isothermal operations the simulations were run for isothermal separations at different temperatures and D/F =1.0 (Runs 1, 2 and 3). The switching times were changed to operate at the optimum port velocity based on the local equilibrium theory in each case. If maximizing PI is desired, there is a slight advantage to operating at the high temperature. Runs 4 to 6 in Table 1 show the simulation results with different heater, cooler and feeds temperatures at D/F =1.0. The raffinate and extract purity increases with the increase in the heater temperature because $u_{B5} >> u_{port}$ (Runs 4 and 5). When F2 has higher temperature than F1 ($T_{F2} \geq T_{F1}$), the raffinate purity increases because $u_{A2} >> u_{A3} \geq u_{port}$ (Runs 5 and 6).

Conclusion

A new design for a thermally assisted SMB system with two-feeds is developed to improve the purity and decrease the solvent usage. The developed design can be easily realized based on the proven SMB technology. The results of this work will provide a guideline to design a thermally assisted SMB with two-feeds.

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