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An optimization-driven novel operation of simulated moving bed chromatographic separation

S.V. Vignesh, K Hariprasad, Pratik Athawale, Sharad Bhartiya *

Department of Chemical Engineering,
Indian Institute of Technology-Bombay, Mumbai - 400 076 India

Abstract: Improvements of conventional SMB operation, such as in Varicol, Modicon, and Powerfeed, have enhanced SMB performance in the past decade. In this work, we propose a novel strategy that incorporates changing internal flow rates and switching periods periodically to enhance flexibility of operation and simultaneously enhance the purity of key product. This mode of operation, called as a dual switching strategy, has been investigated from a modelling perspective with simulation studies to validate the findings. The study incorporates detailed multiobjective optimization problem formulation focusing on performance metrics such as extract purity, recovery and throughput. Unlike the classical SMB processes, dual switching offers a wider scope with its larger degrees of freedom to mutually enhance purity and concentration of key product without the need for SMB configuration modifications. The results reveal a possible fractionating effect on the product side leading to two different purity fractions. Superior performance over the conventional operation has been validated by comparison with classical operation on an SMBC process for separation of glucose and fructose using Ca^{++} exchange resin.

Keywords: Simulated moving bed chromatography, dual switching, multiobjective optimization, glucose-fructose system

1. INTRODUCTION

Chromatographic separations have received significant attention in the pharmaceutical, speciality and fine chemical industry in the making of high purity products and is based on the differing affinities of the mixture constituents to a stationary solid phase. Fixed bed chromatography is a mature batch operation technology for separation of heat-sensitive mixtures or mixtures with similar relative volatilities. While continuous, counter-current operations have the obvious advantage of high productivity and low eluent consumption, physical movement of the solid phase is operationally difficult to accomplish. Simulated Moving Bed Chromatography (SMBC), invented by Broughton and Gerhold Broughton and Gerhold (1961), provides a practical realization of the counter-current flow of the liquid/gas mobile phase and the solid stationary phase.

The SMBC process consists of multiple columns, which are connected in series in a circular manner as shown in Fig. 1. The feed consisting of a mixture of component B (more adsorbed) and A (less adsorbed), and the desorbent streams enter the system, while extract and raffinate streams continuously exit out. Counter-current movement of solid stream is approximated by sequentially switching the inlet and outlet ports of interconnected columns in the direction of fluid flow. Based on the position of columns connected to the feed and desorbent nodes, the SMB is divided into four sections each with a specific function in separating the feed mixture (see Fig. 1). In general, the number of columns in each section may exceed one. By choosing an appropriate switching time interval and flow rates, the preferentially adsorbed species B can be withdrawn at the extract outlet and the less adsorbed species A appears at the raffinate outlet. As seen from Fig. 1, the feed along with the internal flow from section 2 enters section 3, where component B is preferentially adsorbed on the stationary phase, while component A is partly withdrawn at the raffinate outlet and the remaining component A in the internal stream is almost completely adsorbed in Section 4. The desorbent is used to regenerate the adsorbent bed by desorbing component B in the B-rich section 1, a part of which is withdrawn as the extract. At

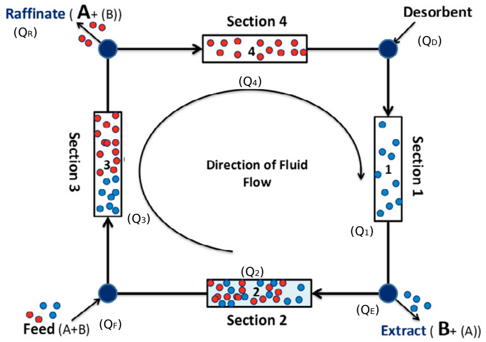

Fig. 1. Schematic of 4 column SMBC unit

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* Corresponding Author: bhartiya@che.iitb.ac.in (Sharad Bhartiya),Tel: +91 22 25767225. Funding from the Department of Science and Technology, India, under Grant number, 13DST05 is gratefully acknowledged.

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the end of switch time, the ports are switched with the feed and desorbent now entering column 4 and column 2 respectively and the respective exits yielding the raffinate and extract. After four such port switches, the original port configuration is obtained and corresponds to one cycle. At a point when the transient concentrations in the columns are identical over the cycle periods, a Cyclic Steady state (CSS) is said to have been reached.

Since the original invention in 1961, numerous modifications that provide improved performance over the classical or conventional SMB have been patented or reported in open literature (Luderman et al., 2000; Zhang et al., 2003; Li et al., 2010). These improvements are a result of incorporating additional flexibility/hardware or degrees of freedom to the SMBC apparatus. The Varicol strategy (Luderman et al., 2000) has unequal number of columns per section of the separation zone and is commercialised by Novasep SAS (France) since it enhances productivity.

Modicon (Schramm et al., 2003) strategy uses the fact that varying the feed concentration within a switching interval could lead to a marked influence on the internal concentration profiles within the column and thereby enable an appropriate shift of impurity fronts for better separation. In the PowerFeed Strategy (Zhang et al., 2003), the degrees of freedom of operation is increased to allow for changing internal flow rates within a switching period t^* thereby offering flexibility of operation. In Feed-Fractionation-SMB (FF-SMB) operational mode, a certain high purity fraction of extract stream is collected and the lean stream is fed back as a recycle to the feed tank. There is a requirement for an extra buffer tank for collection of these recycles whose purity is averaged out over several fractions (Li et al., 2010).

All the above modifications are obtained by addition of new hardware or process elements (for example, a recycle stream or modulation of input concentration or flow rate during a switch) that create new degrees of freedom, which are subsequently leveraged for the process improvement such as enhanced purity or productivity. The current work proposes a radically different operating strategy that creates new operating degrees of freedom in the conventional SMB without requiring any new hardware or process elements. This is brought about by alternating between two sets of flow rates and switch time after every port switch. We term this novel strategy as *Dual switch* operation. Using two sets of operating parameters and alternating between them after every switch doubles the degrees of freedom. These sets of operating parameters are determined using formal model based optimization with the objective of maximizing some SMB performance metric. The proposed approach has been tested by simulations using a benchmark glucose/fructose separation system with the objective of maximizing fructose purity. Simulation results show that upon achieving a dual period cyclic steady state, the fructose-rich extract stream under the dual switching operation yields two distinct fructose rich product cuts at alternate switches: 1) a low purity fructose-rich stream; and 2) a high purity fructose rich stream. At CSS, the high purity cut has a switch-time averaged purity of 99%, which is significantly higher than the maximum switch-time averaged purity achievable in the conventional single switch operation with the same SMB apparatus (96.9%). Moreover, the concentration of the high purity product is significantly higher than the concentration of the product stream in the single switch operation, which is non-intuitive. This suggests that the novel dual operating strategy can be used as a means of process intensification using a conventional SMB apparatus solely by changing the operating procedure. Modulation of flow rates continually through the four sections within a switch period has been proposed by Kloppenburg and Gilles (1999) and has been referred to as time-variable SMB. The flow rate modulation, achieved by a controller, can potentially lead to an improved steady state waveform that aids separation. The current work differs from the above in that the flow rates are maintained at a constant level within a switch period and change only in the subsequent switch to new fixed levels while in the above works the flow rates are modified continually within each switch period (like PowerFeed). The rest of the document is structured as follows: in the next section, a brief overview of the mathematical model used for optimization is presented. Section 3 and 4 present the Dual Switch SMB operation and the corresponding results. Conclusions are presented in Section 5.

2. MATHEMATICAL MODEL OF SMBC

In order to determine optimal operation of the SMB using the proposed dual switch operation, a first principles, 1-dimensional, dynamic model for separation of glucose/fructose, which can describe the spatio-temporal variation in the interconnected columns as well as port switching operations is used (Rajendran et al., 2009). The model uses linear, non-interacting adsorption isotherms for the two species. A linear driving force model and axial dispersion are assumed for the two species. We summarize the model equations here but cite Rajendran et al. (2009); Kawajiri and Biegler (2006) for details. The following notation is used: $c_{ij}(z,t)$, $q_{ij}(z,t)$, $q^*_{ij}(z,t)$ - concentration of the i^{th} component in the j^{th} column in the liquid phase, solid phase, and solid at equilibrium, respectively, in the axial direction z and time t; v_j - axial velocity in the j^{th} column; K_i , k_i, D_i - Henry's constant, mass transfer coefficient and dispersion coefficient for i^{th} species; ϵ - bed porosity; Q_i - internal flow rate in Section i (see Fig. 1); L - column length

Mass balance in liquid phase:

$$\frac{\partial c_{ij}}{\partial t} + \frac{(1-\epsilon)}{\epsilon}\frac{dq_{ij}}{dt} = -v_j\frac{\partial c_{ij}}{\partial z} + D_i\frac{\partial^2 c_{ij}}{\partial z^2} \tag{1}$$

Mass balance in solid phase:

$$\frac{\partial q_{ij}}{\partial t} = k_i\left(q^*_{ij} - q_{ij}\right) \tag{2}$$

$i = 1,\cdots,n_c,$ no. of components$j = 1,\cdots,NC,$ no. of columns

Linear adsorption equilibrium isotherm:

$$q^*_{ij} = K_i c_{ij} \tag{3}$$

Initial condition

$$c_{ij+1}(z,0) = c_{ij}(z,t^*)\,,\ c_{i1}(z,0) = c_{iNC}(z,t^*) \tag{4}$$

Danckwerts boundary condition

$$c_{ij}|_{z=0^-} = c_{ij}|_{z=0^+} - \frac{D_i}{v_j L}\frac{\partial c_{ij}}{\partial z}|_{z=0^+},\quad \left.\frac{\partial c_{ij}}{\partial z}\right|_{z=L} = 0 \tag{5}$$

Desorbent inlet node

$$Q_1 = Q_4 + Q_D, c^{in}_{i1}Q_1 = c^{out}_{i4}Q_4 \tag{6}$$

Extract outlet node

$$Q_2 = Q_1 - Q_E, c^{in}_{i2} = c^{out}_{i1} = c^E_i \tag{7}$$