Computers and Chemical Engineering 84 (2016) 83–95

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Optimal strategies for transitions in simulated moving bed chromatography☆

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

Department of Chemical Engineering, Indian Institute of Technology Bombay, Mumbai 400076, India

ARTICLE INFO

Article history:
Received 6 April 2015
Received in revised form 9 July 2015
Accepted 6 August 2015
Available online 10 September 2015

Keywords:
Simulated moving bed
Chromatography
Nonlinear programming
Optimal transitions

ABSTRACT

Simulated moving bed chromatography (SMBC) has emerged as a significant separation technology in the process industry. SMB operating parameters are chosen to satisfy various performance objectives such as maximization of purity or productivity and the choice of the objective is generally guided by process economics. From an industrial perspective, the SMB must be operated flexibly, so that the same unit can be operated to satisfy different objectives. Transiting from one objective to another entails large transition periods, resulting in an economic loss. We propose use of optimal transitions as an approach to minimizing transition time, reducing use of feed and desorbent during transition as well as reduction in off-specification product relative to a non-optimal, step change approach. Optimal transitions can also be used in recovering from feed upset scenarios. The above methods are demonstrated using simulations on a benchmark SMBC process for separation of glucose and fructose using Ca^{++} exchange resin.

1. Introduction

Chromatography is a separation technique based on the different affinities of components in a mixture with a solid media. In comparison to thermal separation methods like distillation, less energy is consumed in chromatographic operation. Simulated moving bed chromatography (SMBC) process is a technical realization of continuous chromatographic separation known as true moving bed (Sá Gomes and Rodrigues, 2012; Broughton and Gerhold, 1961). SMBC has established itself as a powerful separation technique for high value products in the pharmaceutical and fine chemicals industry (Rekoske, 2001). A salient feature of SMBC relative to other continuous separation techniques, such as distillation, is the cyclic nature of the process, which makes the operation transient in nature. The performance of the SMB is critically dependent on the choice of flow rates and port switching period. This issue has been addressed in literature through optimization of performance objectives such as product purity, feed throughput, recovery and productivity for cyclic steady state operation (Beste et al., 2000; Torres Zuniga and Vande Wouwer, 2014; Heinonen et al., 2014; Sreedhar and Kawajiri, 2014; Yao et al., 2014; Agrawal et al., 2014; Agrawal and Kawajiri, 2012; Dunnebier et al., 2000; García et al., 2006). These different objectives are usually conflicting in nature and the optimal strategy must therefore represent an acceptable trade-off.

From an industrial perspective, the SMB operation must be flexible, so that the same SMB unit is able to satisfy varied performance objectives. Moreover, the SMB should be able to handle changes in feed and product grades. This necessitates transiting from one optimal operating point to another. Such a strategy has been successfully applied in the chemical process industry, notably in product grade transition in polymerization reactors (Padhiyar et al., 2006; Prata et al., 2008). In case of SMB, due to the continuous-discrete nature of the process, transiting from one operating point such as maximum purity to another mode such as maximum throughput is a non-trivial task. The intermediate product obtained during transition between the two operating modes may not meet product specification and thus represents an economic loss (Li et al., 2011). Therefore, there is a need to implement the transition from one cyclic steady state to another in an optimal manner. Such an optimal transition is also imperative to account for feed grade changes so that the operating point can be shifted from the old feed grade to the new feed grade while ensuring that the performance specifications of the separation are not violated. These optimal recipes would then serve as targets to orchestrate these transitions. The need for optimal recipes in the context of start-ups and shut-downs has been demonstrated by Li et al. (2011). Their work shows that the conventional start up procedure of SMB takes considerable time for cyclic steady state (CSS) to be attained and use of dynamic optimization to reduce the startup time is beneficial. Recently, Bentley et al. (2014) have

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☆ An abbreviated version of this paper has been presented at DYCOPS 2013.

* Corresponding author. Tel.: +91 2225767225.
E-mail address: bhartiya@che.iitb.ac.in (S. Bhartiya).

http://dx.doi.org/10.1016/j.compchemeng.2015.08.004

experimentally validated an optimized startup strategy for SMB based on a prediction-correction method (Bentley and Kawajiri, 2013). The authors report an increased productivity and reduced desorbent consumption during the startup experiments, thereby demonstrating the benefits of numerical optimization. In our work, we also use dynamic model based optimization to explore optimal transitions in order to steer the SMB operation from one initial CSS to its target CSS quickly. To the best of the authors' knowledge, optimal transitions between optimal operating points in the context of SMB have not been reported in literature. Furthermore, the current work also addresses issues pertinent to optimally incorporating feed grade changes. All the above cases refer to operating policies in an open-loop. Implementing these in a closed loop using feedback control is not pursued in the current work.

The paper is organized as follows: Section 2 presents a brief overview of the SMBC process and summarizes a first principles model from literature that is used to obtain the results. Section 3 presents optimal cyclic steady state operations for different operation modes. Optimal transitions between these CSS operations are presented in Section 4. Finally, conclusions are presented in Section 5.

2. Simulated moving bed chromatography: an overview

The SMBC process consists of multiple adsorbent-laden columns, which are inter-connected in series in a circular manner as shown in Fig. 1. Feed and desorbent streams continuously enter the system, while extract and raffinate streams exit out. A counter-current movement of the solid adsorbent bed is approximated by sequentially switching the inlet and outlet ports of the inter-connected columns in the direction of fluid flow. According to 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).

The feed stream consists of a mixture of component B (fructose, more adsorbed) and A (glucose, less adsorbed). 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. After lapse of the switching period (t^*), the ports are synchronously switched in the direction of fluid flow. Four port switches constitute one cycle of SMB operation and after sufficient number of cycles, concentration profiles inside the columns over a cycle become identical to those observed in the previous cycle and a cyclic steady state (CSS) is said to have been reached.

A first principles dynamic model of the continuous chromatographic process for separation of glucose/fructose reported in literature (Rajendran et al., 2009; Kawajiri and Biegler, 2006; Leao and Rodrigues, 2004) is used to determine optimal cyclic steady state operation of the SMB as well as obtain optimal recipes for transiting between these cyclic steady states. The model is based on linear and non-interacting adsorption isotherms and includes axial dispersion as well as mass transfer resistance. A summary of the model equations is presented subsequently, with the following notation:

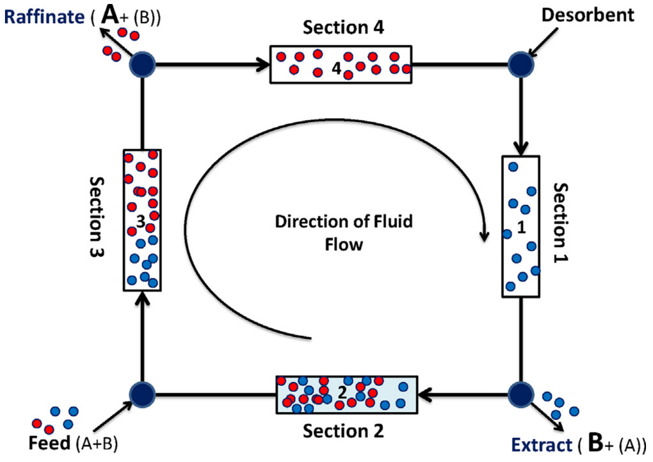

Fig. 1. Schematic of 4 column SMBC unit.

Table 1
SMB simulation model parameters for Eqs. (1)–(5).

Parameter	Values	Parameter	Values
d_c (cm)	2.54	k_i (s^{-1})	0.1
L (cm)	40	ϵ	0.4
$K_{i=fru}$	0.5634	N_{col}	4
$K_{i=glu}$	0.3401	$c^F_{i=glu}$, $c^F_{i=fru}$ (g/l)	30

- c_{ij}, q_{ij} – concentration of the ith component in the jth column in the liquid and solid phases; $q_{ij}{}^*$- equilibrium concentration in the solid phase; t^*- switch duration; v_j – axial velocity in the jth column; K_i, k_i, D_i – Henry's constant, mass transfer coefficient and dispersion coefficient for ith species; ϵ – bed porosity; Q_i – internal flow rate in Section i.

Transport model equations:

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

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

$i = 1, \cdots, n_c,$ the number of components

$j = 1, \cdots, NC,$ the number of columns

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

Initial and boundary conditions:

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

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

Node balances

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

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

$$Q_3 = Q_2 + Q_F; \quad c^{in}_{i3}Q_3 = c^{out}_{i2}Q_2 + c^F_i Q_F \tag{8}$$

$$Q_4 = Q_3 - Q_R; \quad c^{in}_{i4} = c^{out}_{i3} = c^R_i \tag{9}$$

The adsorbent is a strongly acidic cationic resin of gel type (Ca^{2+} form) on which fructose gets preferentially adsorbed relative to glucose. Deionized water is used as the desorbent. Fructose-rich stream is drawn out as extract and is considered as the main product. Model parameters corresponding to the SMBC and the glucose/fructose separation are summarized in Table 1.

3. Optimal cyclic steady state operation of SMBC

Several researchers have presented the optimal cyclic steady state operation of SMBC (Zhang et al., 2002; Subramani et al., 2003; Kawajiri and Biegler, 2006). Here, the objective is to optimize some performance objective like purity or throughput while operating at CSS. In contrast, the main goal of the present work is determining