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Optimization of startup and shutdown operation of simulated moving bed chromatographic processes

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ABSTRACT

This paper presents new multistage optimal startup and shutdown strategies for simulated moving bed (SMB) chromatographic processes. The proposed concept allows to adjust transient operating conditions stage-wise, and provides capability to improve transient performance and to fulfill product quality specifications simultaneously. A specially tailored decomposition algorithm is developed to ensure computational tractability of the resulting dynamic optimization problems. By examining the transient operation of a literature separation example characterized by nonlinear competitive isotherm, the feasibility of the solution approach is demonstrated, and the performance of the conventional and multistage optimal transient regimes is evaluated systematically. The quantitative results clearly show that the optimal operating policies not only allow to significantly reduce both duration of the transient phase and desorbent consumption, but also enable on-spec production even during startup and shutdown periods. With the aid of the developed transient procedures, short-term separation campaigns with small batch sizes can be performed more flexibly and efficiently by SMB chromatography.

1. Introduction

Simulated moving bed (SMB) chromatography as a continuous separation technique has been attracting increasing attention since it was developed by UOP in the early 1960s. Due to significant advantages over conventional batch chromatography, it has found many applications in the last decades in petrochemical, sugar, and fine chemical industries at various production scales. Recently, SMB has been identified as a critical tool in the pharmaceutical industry, especially for the separation of enantiomers using chiral stationary phases. For more details about SMB chromatography and its related subjects, we refer the interested reader to the comprehensive review given by Rajendran et al. [1].

The SMB system is designed as a practical realization of the true moving bed (TMB) operation. The process consists of multiple identical chromatographic columns which are connected to each other to form a closed circle. The two inlets (feed and desorbent) and two outlets (extract and raffinate) divide the unit into four distinct zones fulfilling specific roles for the separation of a binary mixture of A and B. The feed and desorbent are supplied continuously, and meanwhile the less retained component A and the more retained component B are also continuously withdrawn in the raffinate and extract streams, respectively. To mimic the countercurrent movement in TMB, the positions of the four streams are periodically shifted by one column ahead in the direction of the liquid flow after a certain switching period. Due to such a cyclic switching operation along the circularly arranged columns, SMB does not reach a steady state but rather a cyclic steady state (CSS) after startup.

Operating an SMB unit for a given separation task in general undergoes startup, normal production and shutdown periods. For convenience, we refer to the startup and shutdown also as the transient processes throughout the paper. For industrial SMB applications, typically dilute products are produced over startup and shutdown stages. These transient products do not necessarily meet purity requirements specified for the normal products and thus only CSS is used for production. On the other hand, in the academic community significant research efforts also exclusively focus on CSS. Nevertheless, improving the transient performance is always advantageous for SMBs regardless of process scale. For large-volume productions where emergency situations might occur and regular maintenance of columns is indispensable, fast startup and shutdown procedures allow to resume normal

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production quickly and to reduce non-productive duration. In the case of small-scale separation campaigns, very often the same SMB unit is operated repeatedly to process small batches of well-characterized mixtures of different types. This is a rather common circumstance in pharmaceutical production. In this case, the process is subject to frequent startups and shutdowns to realize product changeover. The transient operating time can be also comparable to the production time, causing a significant portion of the feed to be consumed on the transient phases. Obviously, efficient startup and shutdown strategies are particularly helpful in such case. To the best of our knowledge, however, only very few attempts in the open literature have been made to investigate the startup and shutdown problem of conventional SMB and its derivatives. Lim and Ching [2] suggested to pre-load the columns with the feed to reduce the startup time. Xie et al. [3] further enhanced this approach by developing a detailed design procedure of pre-loading and pre-elution for their tandem SMB process for insulin purification. They also designed a shutdown procedure to recover the retained insulin. Both numerical simulations and experimental validation showed satisfactory transient performance. Bae et al. [4,5] examined effects of feed concentration and flow-rate ratio on startup and steady state behaviors of SMB. Abunasser and Wankat [6] performed both startup and shutdown analyses for their single-column chromatographic analogue to SMB, considering that the analogue would be useful in short campaigns. Rodrigues et al. [7] provided a fast model-based startup procedure for their single-column apparatus used for experimentally reproducing the periodic behavior of SMB, reducing the duration of each experimental run significantly. Nevertheless, as pointed out by the authors, the scheme was not directly applicable to a real multicolumn SMB unit since such process relies on the capability of artificially generating a prescribed inlet concentration profile. In addition, although the work by Zenoni et al. [8] was devoted to the development of an on-line system to monitor the composition of the enantiomers of a chiral SMB unit, the authors also emphasized the importance of optimizing startup and shutdown. However, none of the aforementioned contributions explicitly studied the optimal startup and shutdown operation.

Recently, we have proposed a multistage optimal startup strategy for SMB [9]. A specially tailored decomposition solution algorithm was developed to address the intractable dynamic optimization problem. In this paper, we will discuss the multistage startup concept and solution approach in more detail, and extend our previous work by explicitly considering product quality constraints into the optimal startup problem. Based on a binary separation with nonlinear Langmuir isotherm, the performance of the conventional startup and the multistage schemes with and without product quality requirements will be quantitatively compared for the first time, aiming at evaluating them in a systematic manner. Furthermore, the effect of enforcing quality constraints on the optimal operating condition and startup performance is examined. Similarly, the multistage optimal shutdown problem is also studied in this paper. The performance evaluation of various shutdown strategies is performed and their pros and cons are analyzed.

We start this paper by presenting a mathematical model used to quantify the transient behavior of SMB. In Section 3, a brief overview of design methods developed for SMB chromatography is provided, followed by an introduction of the conventional transient operation. Section 4 details the new multistage optimal startup and shutdown regimes, the problem statement and the solution approach. The systematic comparison of different transient operating policies and discussion of the results obtained is given in Section 5. We end with the concluding remarks and perspectives for future work.

2. Mathematical modeling of transient operation

In order to quantitatively characterize the transient dynamics of SMB, an accurate mathematical model capable of capturing both continuous chromatographic separation and periodical port switching is needed. Such a model can be assembled from the global node balances and the dynamic models of single chromatographic columns. By considering the mass balances around the inlet and outlet nodes, one set of node equations yields:
Desorbent node:

$$Q_{IV} + Q_D = Q_I, \quad c_{i,IV}^{out} Q_{IV} = c_{i,I}^{in} Q_I \tag{1}$$

Extract node:

$$Q_I - Q_E = Q_{II}, \quad c_{i,I}^{out} = c_{i,II}^{in} = c_i^E \tag{2}$$

Feed node:

$$Q_{II} + Q_F = Q_{III}, \quad c_{i,II}^{out} Q_{II} + c_i^F Q_F = c_{i,III}^{in} Q_{III} \tag{3}$$

Raffinate node:

$$Q_{III} - Q_R = Q_{IV}, \quad c_{i,III}^{out} = c_{i,IV}^{in} = c_i^R \tag{4}$$

where Q_j ($j = I, II, III, IV$) are the four internal flow-rates, Q_D the desorbent flow-rate, Q_E the extract flow-rate, Q_F the feed flow-rate, Q_R the raffinate flow-rate, $c_{i,j}^{in}$ and $c_{i,j}^{out}$ the liquid concentrations of component i entering and leaving zone j, c_i^E and c_i^R the liquid concentrations of component i at the extract and raffinate outlets, and c_i^F the feed concentration of component i, $i = A, B$.

To model a single column the equilibrium dispersive model [11] was used. In this model the differential mass balance of component i in each column can be written as

$$\frac{\partial c_i}{\partial t} + \frac{1-\epsilon}{\epsilon}\frac{\partial q_i}{\partial t} + v\frac{\partial c_i}{\partial z} = D_{ap,i}\frac{\partial^2 c_i}{\partial z^2}, \quad i = A,\ B \tag{5}$$

with the following initial and boundary conditions

$$c_i(t,z)|_{t=t_0} = c_{i,0} \tag{6}$$

$$D_{ap,i}\left.\frac{\partial c_i}{\partial z}\right|_{z=0} - v(c_i|_{z=0} - c_i^{in}) = 0, \; D_{ap,i}\left.\frac{\partial c_i}{\partial z}\right|_{z=L} = 0 \tag{7}$$

where c_i and q_i are the concentrations of component i in the liquid and solid phases, respectively, v the interstitial liquid velocity, t the time, z the axial coordinate along the column, ϵ the total porosity of the column, L the column length, and c_i^{in} the concentration of component i at the column inlet. The model assumes a local equilibrium between the two phases. The contributions to band broadening due to axial dispersion and mass transfer resistances are lumped into the apparent dispersion coefficients $D_{ap,i}$. For simplicity, the same coefficient was assumed in this work for both components and determined by using

$$D_{ap,i} = \frac{vL}{2N_{NTP}} \tag{8}$$

with N_{NTP} being the number of theoretical plates per column. The adsorption equilibrium of the two components was characterized by the nonlinear competitive Langmuir isotherm

$$q_i(c_A, c_B) = \frac{H_i c_i}{1 + K_A c_A + K_B c_B}, \quad i = A,\ B \tag{9}$$

with H_i being the Henry constants and K_i the thermodynamic coefficients.

For the initial conditions given in Eq. (6), some additional remarks are required. If the model equations presented above are used to describe the startup behavior, the initial time t_0 denotes the starting time of a new separation campaign. When modeling the shutdown process, it should be understood as the time instance at which the shutdown operation begins. For both kinds of problems,