Computers and Chemical Engineering 67 (2014) 121–132

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Using surrogate models for efficient optimization of simulated moving bed chromatography

Suzhou Li [a], Lihong Feng [a], Peter Benner [a,b], Andreas Seidel-Morgenstern [a,c,*]

[a] Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, D-39106 Magdeburg, Germany
[b] Department of Mathematics, Technische Universität Chemnitz, Reichenhainerstraße 41, D-09126 Chemnitz, Germany
[c] Chair of Chemical Process Engineering, Otto-von-Guericke University, Universitätsplatz 2, D-39106 Magdeburg, Germany

ARTICLE INFO

Article history:
Received 6 September 2013
Received in revised form 26 March 2014
Accepted 27 March 2014
Available online 5 April 2014

Keywords:
Simulated moving bed (SMB) chromatography
Surrogate models
Reduced-order modeling
Trust-region algorithm
Optimization

ABSTRACT

A new approach of using computationally cheap surrogate models for efficient optimization of simulated moving bed (SMB) chromatography is presented. Two different types of surrogate models are developed to replace the detailed but expensive full-order SMB model for optimization purposes. The first type of surrogate is built through a coarse spatial discretization of the first-principles process model. The second one falls into the category of reduced-order modeling. The proper orthogonal decomposition (POD) method is employed to derive cost-efficient reduced-order models (ROMs) for the SMB process. The trust-region optimization framework is proposed to implement an efficient and reliable management of both types of surrogates. The framework restricts the amount of optimization performed with one surrogate and provides an adaptive model update mechanism during the course of optimization. The convergence to an optimum of the original optimization problem can be guaranteed with the help of this model management method. The potential of the new surrogate-based solution algorithm is evaluated by examining a separation problem characterized by nonlinear bi-Langmuir adsorption isotherms. By addressing the feed throughput maximization problem, the performance of each surrogate is compared to that of the standard full-order model based approach in terms of solution accuracy, CPU time and number of iterations. The quantitative results prove that the proposed scheme not only converges to the optimum obtained with the full-order system, but also provides significant computational advantages.

1. Introduction

Simulated moving bed (SMB) chromatography is nowadays a powerful technique for the continuous separation of enantiomers using chiral stationary phases. It has been also successfully applied in petrochemical, sugar, and fine chemical industries due to widely recognized advantages over discontinuous batch chromatography. For more specific details regarding SMB chromatography, the reader is referred to the review given by Rajendran et al. (2009). The SMB process is developed as a practical implementation of the true moving bed (TMB) concept. The schematic diagram of a classical four-zone SMB unit is shown in Fig. 1. It consists of multiple chromatographic columns connected to each other to form a closed loop. The two inlets (feed and desorbent) and two outlets (extract and raffinate) divide the unit into four distinct zones with specific roles for the separation of a binary mixture of A and B. The feed and desorbent are supplied continuously, and meanwhile the two product streams are also continuously withdrawn from the raffinate and extract outlets. To simulate the true counter-current movement in TMB, the four streams are periodically advanced by one column ahead in the direction of the liquid flow after a fixed switching period t_s. Due to such a cyclic switching along the circularly arranged columns, SMB does not reach a steady state but rather a cyclic steady state (CSS) after an initial startup stage.

The optimal design and operation of SMB is of crucial importance, since it allows to exploit the full economic potential of the process and helps successful implementation of the concept on the industrial scale. However, this is a challenging task since the process involves periodic nonlinear dynamics and is governed by partial differential equations (PDEs). With respect to the achievement of CSS, two major classes of optimization approaches have been developed, which are outlined schematically in Fig. 2. The sequential approach discretizes only the spatial domain of the PDEs, thus reducing the original model to a system of ordinary

* Corresponding author at: Max Planck Institute for Dynamics of Complex Technical Systems, Sandtorstraße 1, D-39106 Magdeburg, Germany. Tel.: +49 391 6110401; fax: +49 391 6110403.

E-mail addresses: suzhou@mpi-magdeburg.mpg.de (S. Li), feng@mpi-magdeburg.mpg.de (L. Feng), benner@mpi-magdeburg.mpg.de (P. Benner), seidel-morgenstern@mpi-magdeburg.mpg.de (A. Seidel-Morgenstern).

http://dx.doi.org/10.1016/j.compchemeng.2014.03.024
0098-1354/

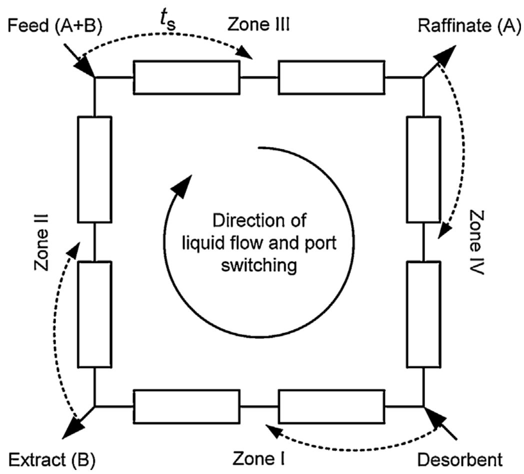

Fig. 1. Schematic representation of a conventional SMB unit with four zones and eight columns.

differential equations (ODEs) or differential algebraic equations (DAEs). The CSS is then achieved by integrating the resulting dynamic model in time for a certain number of switching periods. This approach does not depend on special numerical techniques required by the simultaneous approach except for the solution of differential equations. The resulting nonlinear programming (NLP) problem is small in size and can be addressed directly with general purpose NLP solvers. This strategy also has the ability to couple models exhibiting very detailed and complicated dynamics. With these advantages the method has been used for the optimization of a broad variety of different operating regimes, such as the standard SMB mode (Dünnebier and Klatt, 1999), SMB reactors (Dünnebier et al., 2000), VARICOL (Toumi et al., 2002) and FF-SMB systems (Li et al., 2010). However, the sequential scheme is time-consuming because the CSS integration must be performed at each iteration of the optimization process. In the simultaneous approach, the CSS condition is formulated as an additional equality constraint of the optimization problem. The optimizer determines both the optimal operating parameters and concentration profiles simultaneously within one period. Two variants of the simultaneous approach can be distinguished in the open literature (see Fig. 2(b) and (c)). First, the full-discretization scheme (Biegler et al., 2002) further discretizes the temporal coordinate of the PDEs and the CSS constraint is transformed into a set of algebraic equations. The second variant is implemented based on the framework of direct multiple shooting developed by Leineweber (1999). A large-scale NLP problem arises for both cases. Compared to the sequential approach, the simultaneous formulation eliminates the CSS integration loop and thus is computationally more efficient. Successful applications

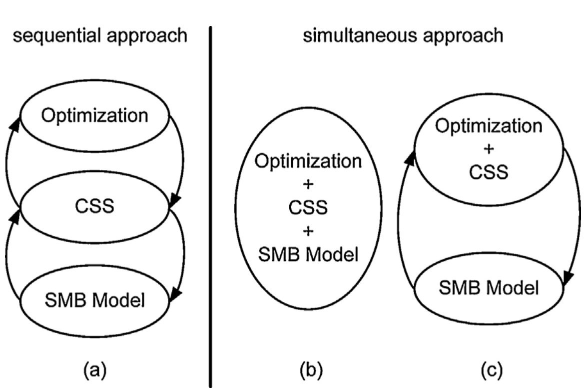

Fig. 2. Sequential approach (a), and simultaneous approach including: (b) full discretization and (c) multiple shooting implementation (Toumi et al., 2007).

of the simultaneous method include the optimization of classical SMB as well as PowerFeed processes (Kawajiri and Biegler, 2006; Toumi et al., 2007). Araújo et al. (2006a) also adopted this method to optimize their single-column models (Araújo et al., 2006b).

It is worth noting that all the methods reviewed above employ a detailed SMB model, either partially or fully discretized, for optimization purposes. The main advantage of using a high-fidelity model is that it can capture more process dynamics and may offer higher accuracy and reliability of results. However, such a model is computationally demanding and constitutes the major challenge for these approaches. For the sequential approach, a high-resolution spatial discretization is often used in order to achieve an accurate approximation to the original PDEs. This results in a large-scale system of differential equations. Integrating such a high-dimensional system repeatedly to satisfy the CSS constraint is expensive. The computational effort is increased if the additional parametric sensitivity equations are solved simultaneously to evaluate the gradients required by the optimization algorithm. On the other hand, the application of the simultaneous scheme to a detailed dynamic model creates a large-scale NLP problem. For such problem, specially tailored optimization algorithms must be used to ensure the satisfactory solution efficiency. Furthermore, the complexity of the optimization problem is further increased when newly emerged SMB variants are optimized, since they include more modeling details and offer additional degrees of freedom.

The challenge mentioned motivates us to use cheap surrogate models for SMB optimization. Surrogate modeling has been proven to be an efficient way to alleviate the computational burden caused by solving expensive engineering design and optimization problems (Forrester and Keane, 2009). It has been gaining great popularity in many areas, in particular in aerodynamics and fluid dynamics. Applications of surrogates to realize efficient design, synthesis and optimization of chemical processes have been also continuously reported recently (Caballero and Grossmann, 2008; Agarwal et al., 2009; Lang et al., 2009; Henao and Maravelias, 2011; Biegler and Lang, 2012; Beck et al., 2012). In the SMB community, however, only few research efforts have been devoted to the development of surrogate models for various purposes. Erdem et al. (2004) applied the balanced model reduction technique to a detailed simulation model to generate a reduced-order model (ROM) that captures the key characteristics of the SMB process. With this computationally efficient ROM, the authors synthesized a real-time model predictive controller for an SMB unit. Vilas and Vande Wouwer (2011) derived a ROM using the proper orthogonal decomposition (POD) method and embedded it in a multi-model predictive control framework. Lübke et al. (2007) proposed a cascadic multilevel algorithm for the fast CSS calculation. The algorithm first employed a surrogate SMB model built by coarse space–time discretization to provide a fast CSS approximation. It then used this rough approximation as the initial condition on finer meshes. It is worth mentioning that Mota and Araújo (2005) developed a novel single-column model with capability to replicate the periodic behavior of SMB. This model can also be considered as an interesting surrogate. It uses only one chromatographic column and its numerical solution is cheap to implement. In addition to the surrogates mentioned above, the TMB model is often used as an approximation to the SMB system for quick analysis and design purposes. This is because the model is continuous and has an easily computable steady state. To the best of our knowledge, however, systematic surrogate-based optimization studies have not been reported for SMB in the open literature.

In this work, we start by developing two different types of surrogate models for the SMB process. The first type of surrogate is obtained by simply employing coarser spatial discretization to the original PDE system. Depending on the mesh resolution used, it has the variable fidelity and is of the model hierarchy type. The second