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Stochastic optimization of simulated moving bed process Sensitivity analysis for isocratic and gradient operation

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Abstract

A random search strategy has been used for designing and optimization of simulated moving bed process (SMB) under isocratic as well as under solvent gradient conditions. The effectiveness of both the process modes has been compared. For predictions of the objective functions, i.e., the minimum of eluent consumption and/or the maximum of the process productivity a mathematical model of the process dynamics has been employed and implemented in the optimization procedure. Four-dimensional space of decision variables corresponding to the flowrates in the SMB zones has been searched in order to find the optimal set of the process parameters. The optimization was constrained to the purity demand in the outlet streams withdrawn in the raffinate and the extract port. The obtained set of random decision variables fulfilling purity constraints was used to construct the operating window of parameters guaranteeing successful separation. For feasible operating points the sensitivity of the purity constraints with respect to the operating parameters has been calculated. The results of calculations indicated that operating conditions, which ensure similar process efficiency, could correspond to different sensitivity of the process constraints. Such an analysis was found to be useful for the selection of process conditions, for which the best trade-off between the process efficiency and its robustness can be achieved. This appears to be particularly important for designing the gradient SMB process, for which robustness of the operating conditions is a factor of a major importance.

In order to improve the efficiency of calculations a modification of the original random search procedure based on the Luus–Jaakola algorithm has been proposed.

Keywords: Stochastic optimization; Simulated moving bed chromatography; Gradient elution

1. Introduction

In the last decade the simulated moving bed (SMB) process has been successfully implemented as a separation technique in the petrochemical, biochemical and fine chemical industries. The SMB is a well-established separation technology basing on continuous chromatography process. The SMB unit was designed as a practical realization of a true moving bed (TMB) where the solid and fluid phases move countercurrently. The general concept of a classical four-zone SMB unit is illustrated schematically in Fig. 1. There are two incoming streams: the feed mixture to be separated ($\dot{V}_F$) and desorbent or eluent ($\dot{V}_D$). Two streams leave the unit, one enriched with the less adsorbable raffinate ($\dot{V}_R$), and one enriched with the more adsorbable extract ($\dot{V}_E$). The four streams divide the unit into four zones (I–IV). Each of these zones contains at least one fixed bed (column) and has to fulfill distinct tasks, i.e., in the zones II and III separations takes place, while in zones I and IV the solid and the fluid phases are regenerated, respectively. The movement of the solid bed is simulated by switching of ports or columns in certain time intervals (Ruthven & Ching, 1989).

The SMB technique is implemented in an industrial scale using the same solvent to prepare the feed and to perform the adsorbent regeneration. This so-called isocratic process is presently well understood (Mazzotti, Storti, & Morbidelli, 1994, 1996, 1997; Migliorini, Mazzotti, & Morbidelli, 1998, 1999; Storti, Masi, Carra, Mazzotti, & Morbidelli, 1989).

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Nomenclature

a, b	linear coefficients in Eqs. (28)–(30)
C	concentration in the fluid phase (vol.%)
EC	eluent consumption (vol. eluent/(vol. product))
H	Henry's constant
k_m	lumped mass transport coefficient (min^{-1})
K_{eq}	equilibrium constant (vol.$^{-1}$)
m	flowrate ratio
$\mathbf{m}$	vector of decision variables
N	total number of iterations in the each pass
N^B	number of fixed beads (columns)
N^C	number of components
N^{end}	number of points in the time grid
N^K	number of cells
NEQ	total number of external passes
NGP	total number of evaluations
NIQ	total number of internal passes
p_H, $p_{K_{eq}}$	parameters in Eqs. (10) and (11)
PR	productivity (vol. product/(vol. solid phase min))
Pu	purity
q	solid phase concentration (vol.%)
$\tilde{q}_i$	solid phase concentration in equilibrium with the local fluid phase concentration (vol.%)
r_H, $r_{K_{eq}}$	parameters in Eqs. (10) and (11)
R	number of points generated in each iteration
S	column cross area (cm^2)
t	time (min)
t^*	switching time (min)
u	superficial velocity (cm/s)
V	column volume (cm^3)
$\dot{V}$	volumetric flowrate (cm^3/min)

Greek letters

β	control parameter for reducing the size of search region
γ	contraction factor for external passes
δ	parameter defining the size of search region for variable $\mathbf{m}$
ε_t	total void fraction
τ	residence time

Subscripts

0	initial values
D	desorbent
E	extract
f	final search region
F	feed
i	component index
j	space interval index
mod	modifier
n_{eq}	n_{eq}th pass of optimization algorithm
n_{iq}	n_{iq}th pass of optimization algorithm
opt	current best value
R	raffinate

Superscripts

K	zone index
N	time interval index

Recently, the idea of modulating of solvent strength in order to increase productivity was introduced to the liquid SMB separation (Abel, Mazzotti, & Morbidelli, 2002, 2004; Antos and Seidel-Morgenstern, 2001, 2002a; Houwig, van Hateren, Billiet, & van der Wielen, 2002; Jensen, Reijns, Billiet, & van der Wielen, 2000). The solvent strength can be modulated in two steps using different solvents at the two inlet ports. The feed is dosed continuously in a relatively weak solvent, whereas as the desorbent a stronger solvent is used (see Fig. 1). Thus, in the classical four zones closed-loop SMB process two distinct levels of internal solvent composition exist which are separated by the two inlet positions. These two characteristic levels of solvent strength can be adjusted by using different amounts of a suitable modifier in the two feed streams. As a result, the components to be separated are more retained in the solvent regeneration zone of the SMB process (zone IV) and more easily eluted in the sorbent regeneration zone (zone I). Recent results of studying this type of two-step gradient SMB process in the closed-loop arrangement demonstrated its potential to reduce significantly the solvent consumption and, thus, to increase product concentrations (Abel et al., 2002, 2004; Antos & Seidel-Morgenstern, 2001, 2002a; Ziomek, Kaspereit, Jeżowski, & Seidel-Morgenstern, 2005).

Design and optimization of such a complex process in an industrial scale can be done by the use of an optimization procedure coupled with an adequate mathematical model of process dynamics.

Recently, stochastic optimization algorithms have been successfully applied for the optimization of isocratic SMB process, e.g., a genetic algorithm was implemented in the multiobjective optimization of a reactive SMB process

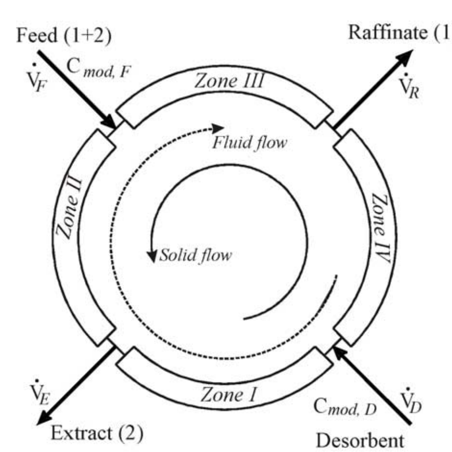

Fig. 1. Scheme of a four-zone SMB unit allowing the implementation of a gradient operation.