



Model-based design and experimental validation of simulated moving bed reactor for production of glycol ether ester



Shan Tie^a, Balamurali Sreedhar^b, Gaurav Agrawal^a, Jungmin Oh^a, Megan Donaldson^b, Timothy Frank^b, Alfred Schultz^b, Andreas Bommarius^a, Yoshiaki Kawajiri^{a,*}

^aSchool of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, USA

^bThe Dow Chemical Company, Midland, MI, USA

HIGHLIGHTS

- A model-based approach is used to optimize the SMBR operation.
- Production rate of SMBR is maximized for a given conversion.
- Model parameters are recalculated using three distinct conversion experiments.
- Model's predictive accuracy is verified outside the experimental conversion range.

ARTICLE INFO

Article history:

Received 22 January 2016

Received in revised form 1 April 2016

Accepted 12 April 2016

Available online 23 April 2016

Keywords:

Simulated moving bed reactor
Model simulation and optimization
Parameter estimation
Experimental validation
Glycol ether ester

ABSTRACT

This work proposes a practical and systematic model-based approach to identify the optimal operating conditions for a simulated moving bed reactor (SMBR). The SMBR operation is applied to an industrial case study for the continuous production of a solvent, propylene glycol methyl ether acetate (DOWANOL™ PMA), which is produced through an acid-catalyzed esterification reaction of 1-methoxy-2-propanol and acetic acid.

The model-based approach is demonstrated by lab-scale SMBR experiments. A multi-objective optimization problem was formulated for developing an SMBR process to maximize the production rate of PMA and the conversion of the esterification reaction simultaneously. In this study, this optimization problem is solved using the epsilon-constrained method and a Pareto plot is presented. The solutions that corresponded to three different values of conversion, 70%, 80%, and 85%, are experimentally validated. The SMBR model that was developed from batch kinetic and single column chromatography experiments demonstrates reasonable agreement with the experimental results. Furthermore, the SMBR experimental data was used to correct the parameters in the model. A validation study at a higher conversion of 95% demonstrates improved predictability of the corrected parameters.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

Within the past decade, there has been growing concern for the impact of anthropological development and progress on the environment. Increasing attention has focused on how chemical processes affect resource consumption and waste generation. Process intensification has gained traction as a way to achieve good product quality and quantity at sustainable production costs and without sacrificing the environment. Process intensification is the engineering of novel methods and equipment to reduce chemical plant footprint and to transform processes to render more

compact, safe, energy-efficient, and environmentally sustainable plants. Such technologies have included new reactors, heat-transfer and mass-transfer devices, hybrid separations, multifunctional reactors, and process-control methods [1]. One solution that has emerged is reactive separation.

Reactive chromatography is a type of reactive separation process rooted in the fundamentals of chromatography. Chromatography is a commonly used technique in chemical engineering that separates component mixtures based on their individual adsorptive properties to the solid phase. The component mixture (feed) is carried through a column by a mobile, liquid phase (desorbent) and the components interact with the stationary, solid phase (adsorbent). Separation of mixtures into individual components occurs due to the relative affinity of each component towards the

* Corresponding author.

E-mail address: ykawajiri@chbe.gatech.edu (Y. Kawajiri).

Nomenclature

A_{cs}	cross-sectional area of the chromatographic column
AA	acetic acid
C	liquid phase concentration (mol/L)
D_{ax}	axial dispersion coefficient (m ² /min)
H	Henry's constant
K_{eq}	equilibrium constant
k_1	forward reaction rate constant (L/mol min)
K_m	mass transfer coefficient (min ⁻¹)
MW	molecular weight
L	column length (m)
N	number
PM	1-methoxy-2-propanol
PMA	propylene glycol methyl ether acetate
q	average solid phase concentration (mol/L)
r	reaction rate (mol/L min)
SMBR	simulated moving bed reactor
t	time (min)
u	interstitial velocity in the column (m/min)
U_L	lower bound on volumetric flow rate (mL/min)
U_U	upper bound on volumetric flow rate (mL/min)
X	conversion
x	axial coordinate

Greek letters

ε	epsilon constraint method
---------------	---------------------------

ε_T	total void fraction
ζ	objective function for SMBR optimization
ξ	conversion
θ	parameter
ν	stoichiometric coefficient
ρ	Tikhonov regularization weighting factor
φ	objective function for parameter estimation

Superscripts and subscripts

comp	component
eq	equilibrium
exp	experiment
rec	recycle stream
i	component (AA, PM, PMA, water)
j	column number (1, 2, 3, 4)
k	experiment data point
m	model parameters ($\varepsilon_T, D_{ax}, K_{eq}, k_1, H_{AA}, H_{PM}, H_{PMA}, H_{water}, K_{AA}, K_{PM}, K_{PMA}, K_{water}$)
D	desorbent stream
Ex	extract stream
F	feed stream
R	raffinate stream

adsorbent. Weakly adsorbing components travel through the column faster and elute earlier whereas the strongly adsorbing components travel slower and elute later.

In a reactive chromatography, the solid phase in addition to being an adsorbent also has catalytic properties. In this operation, when a mixture is fed into the column, the solid phase simultaneously catalyzes product formation and separates the product from its reactants. As a result, the conversion increases because of Le Chatelier's Principle. The dual separation and reaction properties of the solid phase work together such that newly formed products are continuously removed from the reaction locus, thus driving equilibrium-limited reactions to the theoretical conversion of 100%.

The concept of a reactive chromatography process can be incorporated into a simulated moving bed system to create a continuous reactive chromatography process or simulated moving bed reactor (SMBR). The continuous nature of SMBR (Fig. 1) is due to the "simulated" countercurrent flow of the solid phase with respect to the mobile phase by periodically and simultaneously switching the inlet and outlet streams in the direction of liquid flow [2]. There are two inlet ports for the desorbent and feed and two outlet ports for the extract and raffinate. The feed can be composed of a pure, single reactant or a mixture of components. The faster moving components elute from the raffinate while the slower moving components are removed from the extract.

The standard SMBR configuration consists of a minimum of four columns connected in a four-zone design—with one column in each zone. The zones are demarcated by the two inlet ports and the two outlet ports. Each zone's flow rate can be controlled independently yielding four control variables. Zones II and III are mainly responsible for separating the products while zones I and IV regenerate the column by desorbing the adsorbed species. The regular switching of the port positions to simulate the countercurrent motion of the stationary phase is determined by the switching time, the fifth control variable. After start-up, an SMBR system reaches cyclic steady state (CSS) where the concentration profiles

are different among the four zones, but the profile developed within each given zone is identical between cycles. The aforementioned control variables are crucial in determining productivity, product purity and recovery, and solvent consumption and thus require careful optimization for the SMBR operating strategy.

SMBR offers a competitive economic and environmental alternative to conventional sequential integration of batch reactor and separator operations. Specifically, SMBR improves separation resolution, increases productivity, and reduces solvent consumption and waste generation [3].

The advantages of SMBR have attracted attention especially for various industrial applications. Work has been done on the isomerization of glucose to fructose [4,5], hydrogenation of mesitylene [6], isomerization and separation of *p*-xylene [7], synthesis of methyl tertiary butyl ether [8], and esterification reaction involving esters [9,10] and acetic acid [11–13]. Minceva et al.

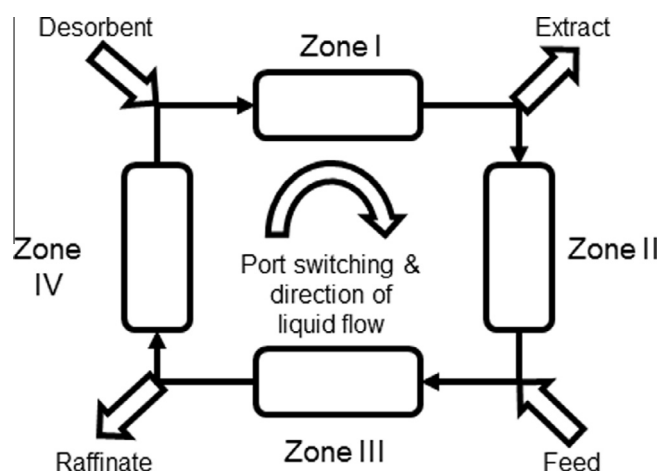


Fig. 1. Schematic of an SMBR operation.

Download English Version:

<https://daneshyari.com/en/article/145406>

Download Persian Version:

<https://daneshyari.com/article/145406>

[Daneshyari.com](https://daneshyari.com)