Computers and Chemical Engineering 106 (2017) 40–56

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Multi-objective optimization of a reactive batch distillation process using reduced order model

P. Swapna Reddy[a,b], K. Yamuna Rani[a,*], Sachin C. Patwardhan[b]

[a] Process Dynamics and Control Group, Chemical Engineering Department, CSIR-Indian Institute of Chemical Technology, Hyderabad 500 007, India
[b] Department of Chemical Engineering, Indian Institute of Technology, Bombay, Maharashtra 400 076, India

ARTICLE INFO

Article history:
Received 22 December 2016
Received in revised form 16 May 2017
Accepted 18 May 2017
Available online 26 May 2017

Keywords:
Reactive batch distillation
First principles model
Reduced order model
Input parameterizations
Multi-objective optimization
Modified version of non-dominated sorting genetic algorithm (NSGA-II)

ABSTRACT

Reactive batch distillation (RBD) processes are highly nonlinear in nature and use of first principles model into the optimization problem demands high computational time. Therefore, a reduced order model for RBD process is proposed which is based on selection of states of prime importance, identification of input state variables, definition of reference trajectories for nominal case, and definition of additional variable transformation to facilitate adaptation of the model to variations in operating conditions. Further, the work focuses on development of a multi-objective optimization formulation for arriving at an optimal operation policy for RBD, and a modified version of Non-dominated sorting Genetic algorithm (NSGA-II) is developed for its solution. The proposed approach is evaluated by application to a simulation case study for production of butyl acetate. The optimization results obtained using the reduced order model are comparable to those obtained with first principles model, while requiring only 1/20th of the time.
© 2017 Elsevier Ltd. All rights reserved.

1. Introduction

Reactive batch distillation (RBD) process is an alternative to a typical reactor and distillation combination. The effect of this combination has the potential to increase conversion, improve selectivity, significantly reduce capital investment and provide additional flexibility. RBD processes are suitable for those chemical reactions where equilibrium limits the conversion to low or moderate levels. In today's competitive market environment, achieving optimal operation of a batch process, such as RBD, is of paramount importance for improving product quality and profitability.

Different strategies have been employed for determination of reflux policies for RBD processes. Venimadhavan et al. (1999) have conceptually developed a novel distillate policy for the RBD process for application to butyl acetate production. Bruggemann et al. (2004) have determined the best reflux policy for butyl acetate production, by carrying out a series of simulation studies and evaluating a profit function consisting of product price and energy costs for each simulation in a RBD process. Systematic optimal operation of RBD processes has been attempted by solving an optimization problem to determine the optimal input profiles off-line with an objective to obtain a product with desired specifications in minimum time. Mujtaba and Macchietto (1997) have discussed the optimization problems of batch distillation columns with reaction by considering polynomial curve fitting techniques. In their study, dynamic optimization problem is formulated for maximum conversion problems and solved for a wide range of operation times. The optimal product yield, optimal reflux profile and optimal heat load profiles obtained for a given purity are fitted with polynomial equations and are used to solve maximum profit problem. Fernholz et al. (2000) have developed an optimal operation policy of a semi-batch reactive distillation column considering esterification of methanol and acetic acid process. The optimization problem was solved by parameterization of manipulated variable profiles as piecewise constant polynomials (control vector parameterization approach) and transformation of the dynamic problem into a static optimization problem solved using nonlinear programming (NLP). The decision variables to the optimization problem are the heat duty *Q*, the feed flow rate of acetic acid, reflux ratio R and the final batch time. The objective function is the maximization of productivity of methyl acetate formed at the end of the batch time. Wajge and Reklaitis (1999) have employed distributed campaign optimization of reactive batch distillation processes for the production of Ethyl acetate. The objective function is formulated for maximum conversion of ethanol subject to purity constraint on the product cut. Giessler et al. (2001) discussed the optimization

* Corresponding author.
E-mail addresses: kyrani@iict.res.in, k_y_rani@yahoo.com (K.Y. Rani).

http://dx.doi.org/10.1016/j.compchemeng.2017.05.017
0098-1354/© 2017 Elsevier Ltd. All rights reserved.

Nomenclature

Abbreviations

AA	Acetic acid
BuOH	Butanol
BuAc	Butyl acetate
FM	Full model
NSGA (II)	Non-dominated sorting genetic algorithm
PAE(z_k)	Percent approximation error
RBD	Reactive batch distillation
ROM	Reduced order model
VLE	Vapor liquid equilibria
VLLE	Vapor liquid liquidequilibria
W	Water

Scalars

A_j	Molar hold up (Kmol) stage j
c	Number of components
h	Time step (Sampling time)
k_f	Forward reaction rate constant (h-1)
Keq	Equilibrium constant
L_j	Liquid molar rate (Kmol/h) stage j
nr_3	Amount of butyl acetate that is produced (Kmol)
P	Pressure (Pa)
$R_{j,i}$	Rate of reaction (hr^{-1}) stage j
R_r	Relative reflux rate
T_j	Temperature corresponding to each tray j
T_s	Switch time
t_f	Final batch time (h)
V	Vapor rate (Kmol/h)
x	Molar liquid composition
y	Molar vapor composition

Greek letters

τ	Scaled time
τ_s	Time scale parameter
γ	Activity coefficient
φ	Phase fraction
Ω	Disturbance in the forward rate constant

problem for the production of ethyl acetate in a batch reactive distillation column, considering the effects of the reaction on the trays, the model preciseness and the type of objective function. Khazraee et al. (2011) developed an operational policy for reactive batch distillation for producing ethyl acetate using differential evolution algorithm. Optimal operation of different types of batch reactive distillation columns i.e. conventional and inverted columns were studied by Edreder et al. (2011) for hydrolysis of methyl lactate to lactic acid, where a dynamic optimization problem is formulated for minimization of the batch time considering piecewise constant reflux ratio and a single interval reboil ratio as the control variables for both the columns.

Majority of the available literature on the optimal operation of RBD processes focus on solving single objective optimization problems by considering decision variables as constant or varying with time. However, in RBD processes, there are conflicting objective functions such as maximum product purity and minimum batch time, which cannot be handled as single-objective optimization problems. Optimization using different objective functions lead to different optimal solutions. A possible remedy for this problem is to pose the optimal operation problem of RBD using multi-objective optimization approach. Multi-objective optimization techniques have been gaining importance recently due to the stringent requirements in process operation in the face of growing competition. Recently Segovia-Hernandez et al. (2015) have presented a review of the optimal design of continuous reactive distillation systems using multi-objective optimization techniques. The review highlights advantages of using multi-objective optimization based approaches over single objective based approaches. Also, in the case of non-reactive semi-batch/batch distillation systems, application of multi-objective optimization have shown promising results (Kim and Smith, 2004; Barakat et al., 2008; Leipold et al., 2009). Thus, it can be expected that use of a multi-objective optimization approach for the developing optimal policy can provide a better handle for predicting performance trade-offs arising due to conflicting operating objectives for a RBD process.

It may be noted that RBD models are highly nonlinear and typically consist of a large number of stiff and coupled differential algebraic equations (DAEs). Solution to the large number of DAE's offers a high computational demand. As a consequence, direct use of these mechanistic models for formulating the optimal control problem requires a very large computation time. Moreover, if there are any initial condition variations or any disturbances, then the optimal operating policy has to be re-calculated for the changed conditions. Regenerating optimal policies is a time consuming exercise because of the high computational effort. Thus, there is a need for developing reduced order models that can cut the computational demand and quickly find a near global optimal policy for the changed operating conditions using the stochastic search techniques.

Development of optimal operation policy for production of Butyl acetate using RBD process is of particular interest in this work. The case studies reported in literature on optimal operational policy of RBD processes include methyl acetate, ethyl acetate and methyl lactate systems, whereas optimal operation of RBD process for Butyl acetate production are rather less in number, since this system has typical heterogeneous and homogenous azeotropes and complex thermodynamic behavior. As a consequence, the resulting optimization problem is computationally expensive. Thus, to reduce the computational complexity arising from direct use of the mechanistic model of the RBD process in the optimization formulations, a reduced order model for RBD is developed in this work. The proposed reduced order model consists of three compartments: condenser compartment, tray section compartment and reboiler compartment. By exploiting features of the RBD process under consideration, a dimensionless time variable is defined. A novel method is developed for approximating the dynamics of the tray section using algebraic function approximations of the state variable profiles that exchange information with the other two compartments in terms of the dimensionless time variable. This results in a significant reduction in the number of model equation and model complexity, which, in turn reduces the computational efforts involved in optimization iterations. Through simulation studies, it is shown that the results obtained using the proposed reduced order model are not significantly different from the results obtained using the full mechanistic model.

The paper is organized as follows: Section 2 provides a brief overview of the system description i.e. generic model of RBD process along with the case study for production of butyl acetate using esterification reaction between butanol and acetic acid. A reduced order model for RBD process is developed in Section 3. Section 4 gives the problem formulation for generating optimal operation policies for RBD process. The results obtained are discussed in Section 5, and conclusions are drawn in Section 6.

2. Generic model of reactive batch distillation process

In the present work, a dynamic model for an n-stage RBD column developed by Patel et al. (2007) has been used for carrying out

Download English Version:

https://daneshyari.com/en/article/6469024

Download Persian Version:

https://daneshyari.com/article/6469024

Daneshyari.com