Dynamic simulation and nonlinear control of a rigorous batch reactive distillation

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ABSTRACT

This work deals with the dynamics and control of a high-purity batch distillation column with chemical reaction. A heterogeneous esterification reaction between the acetic acid and butanol takes place to produce butyl acetate. The process model is formulated considering variable liquid holdup, UNIQUAC model for thermodynamic property predictions, nonlinear Francis weir formula for tray hydraulics, pseudohomogeneous model to represent the reaction kinetics and rigorous energy balance. A structured and simple iterative approach is devised to compute the vapor flows with the fast convergence, under the rigorous energy balance.

The representative column is treated with a distillate policy based on which, the lightest product, water is removed as distillate at the starting of production phase. As a consequence, the column gets progressively richer with the main product, butyl acetate. In addition, almost complete conversion of the limiting reactant is achieved. In order to maintain the product purity at the top, a nonlinear generic model controller (GMC) in two different forms has been proposed. Finally, a comparative closed-loop performance is addressed. It is shown that the control scheme, along with the effective distillate strategy, leads to almost complete conversion of ingredients and high-purity products.

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1. Introduction

Batch processing is used in the chemical industry, especially for development and for seasonal, uncertain, or low-capacity production. Batch distillation columns and batch reactors are the common examples. Their combination in reactive distillation (RD) is a process alternative that has the potential to lower capital and operating costs, and reduce environmental emissions, advantages which have been demonstrated in continuous processing [1].

The concept of reactive or catalytic distillation is not new (first patent in 1921 by Backhaus [2]) but in the recent years its successful applications come into the picture. The research on different aspects of RD column [3], such as process synthesis, modeling and simulation, column hardware design, nonlinear dynamics and closed-loop control, is in progress.

There are two modeling techniques in use for the catalytic distillation processes. They are the equilibrium stage model and the nonequilibrium-based (or rate-based) model. The development of a mathematical model for a reactive distillation column, like other processes, is needed for many reasons [4], such as to understand the column dynamics, to formulate the software sensor, to estimate the state variables, and to synthesize the model-based controllers. It is worth mentioning that the process model should be accurate enough so that it can predict the process dynamics precisely, develop a control scheme that provides high quality closed-loop performance and so on. Motivated by this fact, we develop a rigorous model and an efficient simulation algorithm for a high-purity batch reactive rectifier. An effective distillate policy has been adopted for operating the reactive process.

Control of a batch rectifier is practically a challenging task due to its nonstationary and finite time duration nature of the underlying dynamics. The control of batch distillation with chemical reaction is further complicated because of the additional effects of coupled reaction and separation operations. Most probably, fewer than a half-dozen papers (e.g., [5–7]) reported the nonlinear control of batch reactive rectifier. It is with this intention that the present work has been undertaken.

This work proposes a nonlinear control algorithm that consists of the generic model controller (GMC) and an approximate process model-based state predictor. For the representative process, it is seen that the GMC law requires some additional process information that is not available through direct measurement. For this reason, the state predictor has been developed to compute the unmeasured state(s) required for the GMC scheme. In order to investigate the performance of the proposed controller, one more control strategy, namely ideal GMC, has also been designed. Based on our knowledge, the nonlinear control of such rigorous batch reactive rectifier is not reported in literature.

2. The process

The sample high-purity batch reactive distillation column that has been used for dynamics and closed-loop performance study

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Nomenclature

a_j	activity of the jth component in the liquid phase
C	total number of components
D	distillate rate, mol/min
e	error to the controller
H_n^L	enthalpy of liquid leaving nth tray (J/mol)
H_n^V	enthalpy of vapor leaving nth tray (J/mol)
K_a	equilibrium constant of esterification
K_f	forward reaction rate constant for esterification, mol/gm s
k_n	vapor–liquid equilibrium coefficient with respect to nth tray
L_n	liquid flow rate leaving nth tray, mol/min
M_{cat}	mass of the catalyst, gm
m_D	molar holdup in the reflux accumulator, mol
m_n	molar holdup on nth tray, mol
n_T	top tray
P^0	pure component vapor pressure, Pa
P_t	total pressure, Pa
q	area parameter for the UNIQUAC equation
Q_n	heat loss from nth tray (J/min)
r	volume parameter for the UNIQUAC equation
R	reflux rate, mol/min
r_j	reaction rate of component j, mol/s
S_n^L	the molar flow of liquid side stream leaving nth tray (mol/min)
S_n^V	the molar flow of vapor side stream leaving nth tray (mol/min)
T	temperature
u	manipulated input for the GMC scheme
V_n	vapor flow rate leaving nth tray, mol/min
$V_{n_T} y_{n_T,j}$	component (j) vapor flow rate leaving top tray (n_T), mol/min
$x_{B,j}$	mole fraction of the jth component in the bottoms
$x_{D,j}$	mole fraction of the jth component in the distillate
$x_{DSP,j}$	set point value of $x_{D,j}$
x_j	mole fraction of the jth component in the liquid phase
$\hat{x}$	predicted x
y_j	mole fraction of the jth component in the vapor phase
Z_n	composition of feed entering nth tray

Greek letters

γ_j	activity coefficient of jth component
δ_j	stoichiometric coefficient of jth component
ε	tolerance limit

is shown in Fig. 1. It operates at atmospheric pressure and has a total of 15 trays, including the reboiler and total condenser. The trays are counted from bottom to top; reboiler is the 1st tray and condenser the 15th tray. The column consists of three sections, namely rectifying section (12th to 14th tray), reactive zone (5th to 11th tray) and stripping section (2nd to 4th tray).

2.1. Reaction kinetics

The representative column is a heterogeneously catalyzed process and it produces n-butyl acetate (BuAc) and water (H_2O) by the esterification of n-butanol (BuOH) with acetic acid (HAc). The reversible reaction is given as:
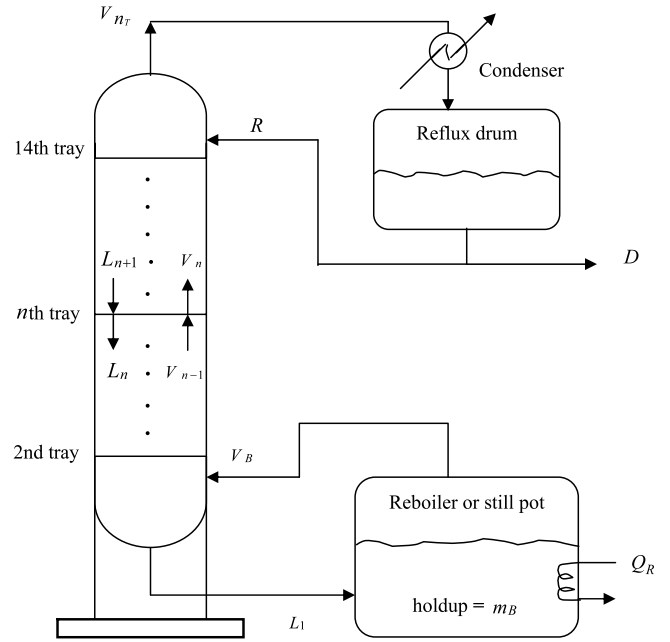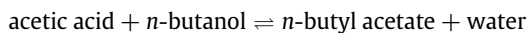
acetic acid + n-butanol $\rightleftharpoons$ n-butyl acetate + water

Fig. 1. Schematic representation of the batch reactive distillation.

Table 1
Kinetic data for the PH model.

K_f^0	3.3856×10^6 mol/gm s
E_f	70.660×10^3 J/mol
K_a^0	3.3405
E_a	-3.5817×10^3 J/mol
M_{cat}	2000 gm/tray

Component number :	(1)	(2)	(3)	(4)
Boiling point (°C) :	118.1	117.9	126.3	100.

As mentioned, there are three sections in the column. The rectification zone and stripping zone operate exactly as a nonreactive distillation column, purifying top and bottom streams. n-Butyl acetate is formed in the reaction zone. For the esterification reaction, the pseudohomogeneous (PH) model has been used. The catalyst, namely Amberlyst-15, has been placed in the reactive zone. The PH model [8] has the following form:

$$r_j = m\frac{\mathrm{d}x_j}{\mathrm{d}t} = \delta_j M_{cat} K_f \left(a_{\mathrm{HAc}} a_{\mathrm{BuOH}} - \frac{1}{K_a} a_{\mathrm{BuAc}} a_{\mathrm{H_2O}} \right) \tag{1}$$

where,

$$a_j = x_j \gamma_j. \tag{2}$$

The temperature dependency of the rate constants K_j is expressed by the Arrhenius equation:

$$K_j = K_j^0 \exp(-E_j/RT). \tag{3}$$

The kinetic data for the PH model are reported in Table 1. The UNIQUAC model is used to determine the activity coefficients in the liquid phase. Values of UNIQUAC parameters and Antoine constants are documented in Table 2.

2.2. Dynamic model development

In the present study, a fundamental model for a batch reactive rectifier is derived. The following assumptions have been adopted:

- Negligible tray vapor holdups
- Variable liquid holdup in each tray
- Perfect mixing and equilibrium on all trays