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Nonlinear state estimation and control of a batch reactive distillation

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ABSTRACT

This paper deals with the advanced adaptive control of a batch reactive distillation (RD) column for the production of ethyl acetate. The nonlinear adaptive control law consists of the generic model controller (GMC) and an adaptive state estimator (ASE). In the first part of the present work, the design approach of the ASE scheme in two different forms, namely ASE1 and ASE2, has been addressed for a batch reactive rectifier. The predictor model of both the ASE estimators includes only a component mole balance equation around the condenser-reflux drum system and an extra state equation having no dynamics, and therefore, there is a large process/predictor mismatch. In presence of this structural discrepancy, the adaptive estimation schemes compute the imprecisely known parameters quite accurately based on the measured distillate composition under initialization error, disturbance and uncertainty. In the subsequent part, the adaptive GMC–ASE1 control structure has been formulated for the sample reactive column. This nonlinear control strategy shows comparatively better closed-loop performance than the gain-scheduled proportional integral (GSPI) controller due to the exponential error convergence capability of the estimation scheme and the high-quality control of the GMC law.

1. Introduction

It is well-known that the distillation columns and chemical reactors are among the most important units used in the chemical and petroleum industries. Reactive distillation (RD) is an innovating process which combines both distillation and chemical reaction into a single unit. Therefore, the RD technology offers many benefits as well as restrictions over the conventional sequential method of reaction followed by distillation or other separation approaches. Reduced capital cost, higher conversion, improved selectivity, lower energy consumption, scope for difficult separations and avoidance of azeotropes are a few of the potential advantages offered by the reactive distillation. Among the key restrictions for the substitution of conventional reactor–separator systems by reactive distillation are the relative volatility of reactants and products, and that the necessary conditions for the reaction must match those of distillation.

Due to the combination of reaction and separation, reactive distillation exhibits complex behaviours [1], such as steady state multiplicity, process gain sign changes (bidirectionality) and strong interactions between process variables. These complexities make reactive distillation process control extremely difficult. Moreover, a RD column offers more limited flexibility than a traditional reactor-–separator process because of the smaller number of manipulated variables available for adjustment.

Research on various aspects of RD column [2], such as modeling and simulation, process synthesis, column hardware, nonlinear dynamics and control etc., is in progress. Most of the literature papers available on reactive distillation are based on steady state conditions including process design (e.g., [3,4]) and the analysis of multiple steady states (e.g., [5–10]). Study on reactive distillation modeling and dynamic simulation (e.g., [11–14]) has also been performed, but a relatively small amount of research work has been reported on the control of RD columns.

Most of the publications on closed-loop control of RD columns deal with the linear control schemes including conventional proportional integral (PI) controller (e.g., [7,15–22]) and model predictive controller (MPC) (e.g., [1,23,24]). Roat et al. [25] presented the inadequacies of conventional linear multi-loop controllers and highlighted the need for more advanced controllers designed within the framework of nonlinear control science. A limited number of papers dealing with the advanced nonlinear control of continuous reactive distillation have appeared in open literature (e.g., [26–30]).

Control of a batch rectifier is really a difficult task owing to its nonstationary and finite time duration nature of the underlying dynamics. Again, batch reactive distillation column control is more

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Nomenclature

C	number of components
d	measurable disturbance vector of dimension q
D	distillate flow rate (mol/min)
H_B^L	enthalpy of the reboiler liquid (kJ/kmol)
$\dot{H}_B^L$	time derivative of H_B^L
H_B^r	heat of reaction in the reboiler (kJ/kmol)
H_B^V	enthalpy of boil-up vapour (kJ/kmol)
H_D^L	enthalpy of the reflux drum liquid (kJ/kmol)
H_n^L	enthalpy of a liquid stream leaving nth tray (kJ/kmol)
$\dot{H}_n^L$	time derivative of H_n^L
H_n^r	heat of reaction in nth tray (kJ/kmol)
H_n^V	enthalpy of a vapor stream leaving nth tray (kJ/kmol)
i	component index
$K_{n,i}$	vapour–liquid equilibrium coefficient for ith component on nth tray
K_P	process gain
L_n	flow rate of an internal liquid stream leaving nth tray (kmol/min)
m_B	liquid holdup in the still pot (kmol)
$\dot{m}_B$	time derivative of m_B
$\dot{m}_B\dot{x}_{B,i}$	time derivative of the multiplication of m_B and $x_{B,i}$
m_D	liquid holdup in the reflux accumulator (kmol)
$\dot{m}_D$	time derivative of m_D
$\dot{m}_D\dot{x}_{D,i}$	time derivative of the multiplication of m_D and $x_{D,i}$
m_n	liquid holdup on nth tray (kmol)
$\dot{m}_n$	time derivative of m_n
$\dot{m}_n\dot{x}_{n,i}$	time derivative of the multiplication of m_n and $x_{n,i}$
n_T	total number of trays
Q_C	condenser duty (kJ/min)
Q_R	reboiler duty (kJ/min)
r	rate of reaction (kmol/(L min))
R	reflux flow rate (kmol/min)
R_S	steady state value of R (kmol/min)
u	input vector of dimension m
V_B	vapour boil-up rate (kmol/min)
V_n	flow rate of a vapour stream leaving nth tray (kmol/min)
$V_{nT}y_{nT,i}$	component (i) vapour flow rate leaving top tray (kmol/min)
$\dot{V}_{nT}\dot{y}_{nT,i}$	time derivative of $V_{nT}y_{nT,i}$
$\hat{V}_{nT}\hat{y}_{nT,i}$	estimated value of $V_{nT}y_{nT,i}$
x	state vector of dimension n
$\hat{x}$	estimated x
$x_{B,i}$	composition of component i in the still pot, mol fraction
$x_{D,i}$	composition of component i in the distillate, mol fraction
$\hat{x}_{D,i}$	estimated $x_{D,i}$
$x_{DSP,i}$	set point value of $x_{D,i}$, mol fraction
$x_{D0,i}$	nominal operating value of $x_{D,i}$ (=$x_{DSP,i}$), mol fraction
$\dot{x}_{D,i}$	time derivative of $x_{D,i}$
$x_{n,i}$	composition of component i in a liquid stream leaving nth tray, mol fraction
y	measured variable vector of dimension n
$y_{B,i}$	composition of component i in the boil-up vapour, mol fraction
$y_{n,i}$	composition of component i in a vapour stream leaving nth tray, mol fraction
y_{SP}	set point value of y
Z	state (true + augmented) vector of dimension 2n
$\hat{Z}$	estimated Z

Greek letters

ε_n	volume of the liquid holdup on nth stage
γ_i	stoichiometric coefficient for the ith component
θ	model parameter vector of dimension n

challenging because of the additional effects of coupled reaction and separation operations. Batch distillation column is an integrating system; during the operation the depletion of light components with time takes a role somewhat like a ramp load and produces a control problem. In such a case, the controller gain must be increased precisely during the batch operation. For this purpose, a gain-scheduled proportional integral (GSPI) controller has been devised in this study.

It is interesting to investigate the nonlinear control performance of a batch reactive distillation. Based on our knowledge, fewer than a half-dozen papers (e.g., [31,32]) reported the nonlinear control of batch reactive rectifier. Two major contributions of the present work are highlighted in the following. (i) It is true that most of the nonlinear estimation schemes involve significant design complexity. The large predictor model and the complex structure of the closed-loop estimator complicate the overall design. To reduce the design complexity as well as computational load, in this study, an adaptive state estimator (ASE) [33,34] has been developed for the ethyl acetate batch reactive column. This estimator has simple structure and the predictor model includes only component mole balance equation around the condenser–reflux drum system and an extra state equation with no dynamics. We must note that the proposed ASE approach only estimates the states (true and augmented) as per the controller requirements. Like other estimation algorithms, it does not compute all the process states. (ii) Second, an adaptive control law, consisting of the generic model controller (GMC) and ASE, has been synthesized for the example batch column. The proposed control structure provides high-quality performance mainly due to the exponential error convergence capability of the ASE estimator. To the best of our knowledge, the design technique of the GMC–ASE control strategy for the batch reactive rectifier is a new one.

This article is arranged as follows. First, a review of the GMC–ASE control structure is presented. Then, a batch reactive rectifier for the production of ethyl acetate by the esterification of ethanol with acetic acid is briefly described. In the next, the nonlinear adaptive controller has been formulated within the framework of GMC law. Then, the ASE scheme has been developed in two different forms, namely ASE1 and ASE2. The GSPI control strategy is also presented in brief. Subsequently, the simulation results section includes the tracking performance of the ASE estimators followed by a comparative closed-loop control performance between the GMC–ASE1 and the GSPI controller. Finally, the conclusion and perspectives of the present work are emphasized.

2. Nonlinear adaptive control structure

The adaptive control algorithm consists of the nonlinear generic model controller and an adaptive state estimator. The closed-loop system having different controller elements and the process is shown in Fig. 1. In the following, the adaptive controller is presented in generalized form.

2.1. Generic model control

In nonlinear modeling of dynamic processes [35], it may be considered that the system is nonlinear in the states, disturbances and

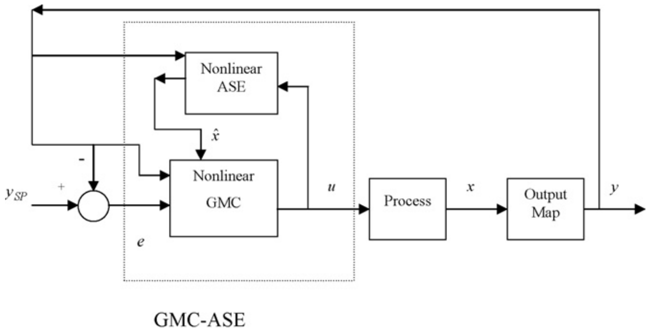

Fig. 1. Block diagram for the nonlinear adaptive control algorithm.

control variables but linear in the model parameters such that:

$$\begin{aligned} &\dot{x} = f(x, d)\theta + g_1(u, x, d) \\ &y = cx \end{aligned}, \tag{1}$$

where the state $x \in \Re^n$, the model parameter $\theta \in \Re^n$, the measurable disturbance $d \in \Re^q$, and the input $u \in \Re^m$. Moreover, f and g_1 are matrices of nonlinear functions. It is assumed that all states are measurable and c (coefficient matrix) is a unity matrix.

From the basic principle of GMC [36], the following control law can be derived [35] as:

$$f(x, d)\theta + g_1(u, x, d) - K_1 e - K_2 \int_0^t e dt = 0, \tag{2}$$

where e is the error ($= y_{SP} - y$) to the controller, y_{SP} is the set point value of the output y, and K_1 and K_2 are diagonal $n \times n$ tuning parameter matrices. Eq. (2) implies that the GMC algorithm comprises of the dynamic modeling equation(s) that directly correlates the controlled variable(s) and corresponding manipulated variable(s), proportional action term and integral action term. If g_1 is linear with respect to u, then one can write $g_1(u,x,d) = b(x,d)u$. Accordingly, Eq. (2) yields:

$$u = (b(x, d))^{-1} \left[K_1 e + K_2 \int_0^t e dt - f(x, d)\theta \right] \tag{3}$$

The values of the elements of tuning parameter matrices can be found out based on the following relationships given by Signal and Lee [37] as:

$$\begin{cases} K_{1(i,i)} = \dfrac{2\tau_{1i}}{\tau_{2i}} \\ K_{2(i,i)} = \dfrac{1}{\tau_{2i}^2} \end{cases}, \tag{4}$$

where τ_{1i} and τ_{2i} determine the shape and speed of the desired closed-loop trajectory (the reference trajectory), respectively. The reference trajectory gives pseudo-second order response for a step change in the set point. However, Yamuna and Gangiah [38] confirmed that the above relationships could be applied to compute the specified response accurately. Once the values of τ_{1i} and τ_{2i} are obtained, then K_1 and K_2 can be calculated from Eq. (4).

2.2. *Adaptive state estimation*

In practice, there are usually two types of mismatch, structural mismatch and parameter mismatch. The structural mismatch exists when there is a difference between the actual plant model and the predictor model. The parameter mismatch occurs when the numerical values of parameters in the predictor model differ with the process values. The effects of the structural discrepancy on the closed-loop performance can be reduced if the imprecisely known parameters are continuously updated.

In the present study, the model parameters in Eq. (1) are supposed to be time varying. Here, a nonlinear observer proposed by Farza et al. [33,34] is designed to estimate the poorly known parameters of the reactive batch rectifier. It is also assumed that the parameter dynamics in the nonlinear system (Eq. (1)) obey the following general first-order equation:

$$\dot{\theta} = g_2(u, x, d) + \varepsilon, \tag{5}$$

where g_2 is a nonlinear function and ε is an unknown function that may depend on x, θ, u, d, noise, and so on. The assumptions that have been made are: ε is an unknown but bounded function and the disturbance d with its time derivative are also bounded.

The nonlinear system Eqs. ((1) and (5)) can be expressed in the following condensed form as:

$$\begin{cases} \dot{Z} = F(x, d)Z + G(u, x, d) + \bar{\varepsilon} \\ y = CZ \end{cases}, \tag{6}$$

where $Z = \begin{bmatrix} x \\ \theta \end{bmatrix}$, $F(x, d) = \begin{bmatrix} 0 & f(x, d) \\ 0 & 0 \end{bmatrix}$, $G(u, x, d) = \begin{bmatrix} g_1(u, x, d) \\ g_2(u, x, d) \end{bmatrix}$, $\bar{\varepsilon} = \begin{bmatrix} 0 \\ \varepsilon \end{bmatrix}$ and $C = \begin{bmatrix} I_n, & 0 \end{bmatrix}$, with I_n the $n \times n$ identity matrix. f is an $n \times n$ matrix which is differentiable and the corresponding partial derivative is continuous.

According to Farza et al. [33], the nonlinear adaptive observer can be used to track the vector Z as follows:

$$\dot{\hat{Z}} = F(y, d)\hat{Z} + G(u, y, d) - \Gamma^{-1}(y, d)S^{-1}C^T(C\hat{Z} - y), \tag{7}$$

where

(i) $\hat{Z} = \begin{bmatrix} y \\ \hat{\theta} \end{bmatrix} \in \Re^{2n}$, and $\hat{\theta} \in \Re^n$.

(ii) $\Gamma(y, d) = \begin{bmatrix} I_n & 0 \\ 0 & f(y, d) \end{bmatrix}$.

(iii) S is the unique symmetric positive-definite matrix which satisfies the algebraic Lyapunov equation.

The gain of the estimator is obtained as:

$$\Gamma^{-1}(y, d)S^{-1}C^T = \begin{bmatrix} 2\alpha I_n \\ \alpha^2 f^{-1}(y, d) \end{bmatrix} \tag{8}$$

where, $\alpha > 0$ is a design parameter [39].

It is obvious from Eq. (8) that only a single tuning parameter α is involved in the estimator. When $\varepsilon = 0$, the convergence of the observer error is an exponential one. In the case where $\varepsilon \neq 0$, the asymptotic error can be made arbitrarily small by choosing a sufficiently large value of α. However, a very large value of α may make the observer sensitive to noise. Thus, the choice of α is a compromise between fast convergence and sensitivity to noise.

3. The process

The sample batch reactive distillation column [31,40] that has been used for closed-loop performance study is shown in Fig. 2. It has total eight trays, excluding the reboiler and total condenser. The trays are counted from bottom to top; bottom tray is 1st tray and top tray is eighth tray. Without clouding the picture with the specific complexities that can occur in some real chemical systems, simple vapor–liquid equilibrium, reaction kinetics and physical properties have been considered. The key objective of the present work is to investigate the closed-loop process dynamics with the application of control algorithms.

The concerned process produces ethyl acetate and water by the esterification of ethanol with acetic acid:

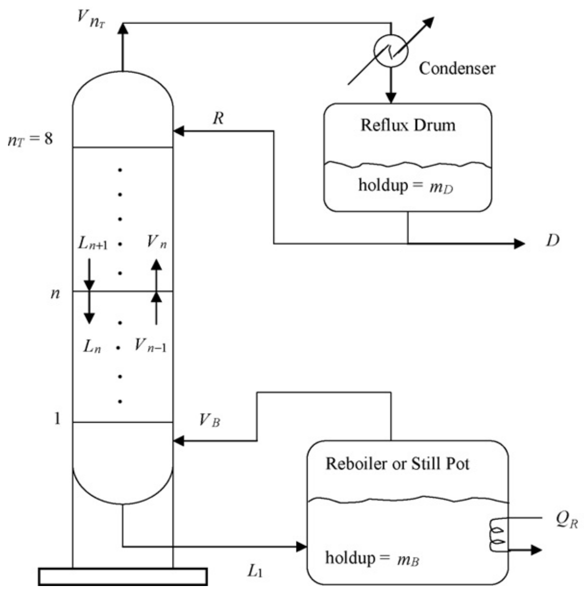

Fig. 2. Schematic representation of the batch reactive distillation.

	acetic acid +	ethanol ⇄	ethyl acetate +	water
Boiling (K) → point	391.1	351.5	350.3	373.2

The reaction is slightly endothermic and takes place in the liquid phase. For the ethanol esterification reaction, the kinetic data presented by Mujtaba and Macchietto [40] are listed in Table 1.

The main product, ethyl acetate, is the lightest component in the mixture. The continuous withdrawal of ethyl acetate as distillate shifts the chemical equilibrium further to the right and consequently, the reactant conversion is improved. The example process is discussed in detail in Appendix. The model and system characteristics are reported in Table 1.

4. Controller synthesis for the batch reactive rectifier

The control objective is to produce the overhead product with a specified purity of ethyl acetate. The manipulated input is the reflux flow rate. As mentioned, the reflux drum holdup is remained almost unchanged by the employment of a traditional P-only controller.

In the present study, a nonlinear adaptive control algorithm has been developed for a multi-component reactive batch distillation column. To examine the control performance of the proposed adaptive controller, a comparative study has been carried out between the GMC–ASE and the gain-scheduled proportional integral control structure.

Table 1
Column specifications and reaction kinetic data.

Column specifications	
System	Acetic acid/ethanol/ethyl acetate/water
Total feed charge (kmol)	30.0
Feed composition (start-up), mol fraction	0.45/0.45/0.0/0.1
Tray holdup (start-up) (kmol)	0.075
Reflux drum holdup (kmol)	0.6
Heat input to the still pot (kJ/min)	3200
Distillate flow rate (production phase) (mol/min)	0.06
Distillate composition (steady state), mol fraction	0.9344
Kinetic data	
Rate of reaction (kmol/(L min)): $r = k_1 c_1 c_2 - k_2 c_3 c_4$	
Rate constants: $k_1 = 4.76 \times 10^{-4}$; $k_2 = 1.63 \times 10^{-4}$	
Where c_i = concentration (kmol/L) for the *i*th component	

4.1. Nonlinear adaptive control system

As stated earlier, the adaptive GMC–ASE control law is derived by combining the generic model controller and an adaptive state estimator. In the following, the adaptive control elements are designed based on the theories presented in Section 2.

4.1.1. Generic model controller

The component mole balance around the condenser–reflux drum system yields:

$$\dot{m}_D \dot{x}_{D,i} = V_{nT} y_{nT,i} - (R+D)x_{D,i} + \gamma_i r_D \varepsilon_D \tag{9}$$

In the closed-loop simulation study, a level controller (P-only) is employed to maintain the liquid holdup in the reflux drum at a desired value. The variation of holdup is so small (±1.0%) that it is reasonable to assume constant m_D. Accordingly, the above equation gives:

$$\dot{x}_{D,i} = \frac{V_{nT} y_{nT,i} - (R+D)x_{D,i} + \gamma_i r_D \varepsilon_D}{m_D} \tag{10}$$

Using Eq. (2) and simplifying, the GMC control law can be obtained in the following form for the representative process:

$$R = \frac{V_{nT} y_{nT,i} + \gamma_i r_D \varepsilon_D - m_D \left(K_1 e + K_2 \int_0^t e dt \right)}{x_{D,\,i}} - D, \tag{11}$$

where $e = x_{DSP,i} - x_{D,i}$, and $x_{DSP,i}$ is the set point value of $x_{D,i}$. To implement the nonlinear GMC controller (Eq. (11)), the information on the component vapour flow rate leaving top tray ($V_{nT} y_{nT,i}$), a poorly known parameter, is required in each time step. So, there is a need to estimate that parameter.

The values of GMC tuning parameters are selected based on the guidelines given in Section 2 as: $K_1 = 20$ and $K_2 = 0.000012$. Notice that to obtain satisfactory controller tuning parameters for the closed-loop batch distillation operation, we need to follow the conventional start-up procedure [41].

4.1.2. Adaptive state estimator

In order to estimate $V_{nT} y_{nT,i}$, the GMC control strategy includes the ASE scheme forming the GMC–ASE control structure. The ethyl acetate composition in the distillate ($x_{D,i}$, where $i = 3$ for ethyl acetate) is assumed as the measured variable (true state), whereas $V_{nT} y_{nT,i}$ ($i = 3$) is considered as the extra state having no dynamics. Although $x_{D,i}$ is obtained through direct measurement, that composition is also estimated in the ASE to compute the residual, $\hat{x} - x$ (=estimated value − measured value).

In the present work, the adaptive state estimator has been designed in two different forms, namely ASE1 and ASE2. The ASE1 has only one extra state ($V_{nT} y_{nT,i}$) and the ASE2 includes two extra states ($V_{nT} y_{nT,i}$ and r_D).

4.1.2.1. Design of ASE1. The predictor model, which is an integral part of the ASE1 scheme, consists of the component mole balance equation around the condenser–reflux drum system and an extra state equation with no dynamics. It has the following representation:

$$\begin{cases} \dot{x}_{D,i} = \dfrac{V_{nT} y_{nT,i} - R x_{D,i} - D x_{D,i} + \gamma_i r_D \varepsilon_D}{m_D}, \\ V_{nT} \dot{y}_{nT,i} = 0.0 \end{cases} \tag{12}$$

where $V_{nT} \dot{y}_{nT,i} = d(V_{nT} y_{nT,i})/dt$. The final structure of the ASE1 estimator can be derived in matrix form by combining Eqs. (7), (8) and

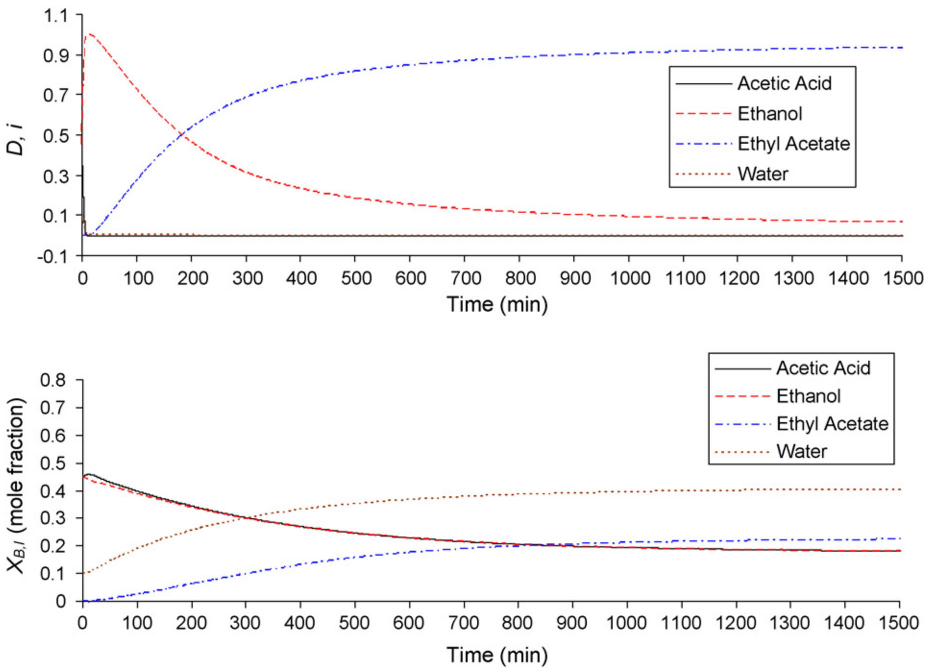

Fig. 3. Open-loop process dynamics at the start-up phase under total reflux condition with having reaction (no reaction only in the first 11 min).

(12) as:

$$\begin{bmatrix}\dot{\hat{x}}_{D,i}\\ \dot{\hat{V}}_{nT}\dot{\hat{y}}_{nT,i}\end{bmatrix} = \begin{bmatrix}0 & \dfrac{1}{m_D}\\ 0 & 0\end{bmatrix}\begin{bmatrix}\hat{x}_{D,i}\\ \hat{V}_{nT}\hat{y}_{nT,i}\end{bmatrix} + \begin{bmatrix}\dfrac{-Rx_{D,i}-Dx_{D,i}+\gamma_i r_D\varepsilon_D}{m_D}\\ 0\end{bmatrix} - \begin{bmatrix}2\alpha_1\\ \alpha_2^2 m_D\end{bmatrix}[\hat{x}_{D,i}-x_{D,i}], \qquad (13)$$

where $\hat{x}_{D,i}$ and $\hat{V}_{nT}\hat{y}_{nT,i}$ are estimates of $x_{D,i}$ and $V_{nT}y_{nT,i}$, respectively. In the above estimator structure, α_1 and α_2 are the tuning parameters. It is true that the dynamics of $x_{D,i}$ and $V_{nT}y_{nT,i}$ are not same. Hence, it is better to estimate $x_{D,i}$ and $V_{nT}y_{nT,i}$, using different tuning parameters, respectively. The values of these parameters have been determined based on the guidelines suggested by Farza et al. [34] as: $\alpha_1 = 110$ and $\alpha_2 = 20$.

The estimator has been used here to compute $x_{D,i}$ and $V_{nT}y_{nT,i}$ for ethyl acetate ($i = 3$) only. It is important to mention that the estimated extra state ($\hat{V}_{nT}\hat{y}_{nT,i}$) and the measured true state ($x_{D,i}$) have been used in Eq. (11) to compute the GMC responses.

4.1.2.2. Design of ASE2. In this case, the predictor model has the following structure:

$$\begin{aligned}\dot{x}_{D,i} &= \frac{V_{nT}y_{nT,i} - Rx_{D,i} - Dx_{D,i} + \gamma_i r_D\varepsilon_D}{m_D}\\ \dot{V}_{nT}\dot{y}_{nT,i} &= 0.0\\ \dot{r}_D &= 0.0\end{aligned} \qquad (14)$$

Since this estimator aims to compute mainly two partially known parameters ($V_{nT}y_{nT,i}$ and r_D) based on a single measured variable ($x_{D,i}$), there is a need to partition the state estimator into the following two square subsystems.

Subsystem-1

$$\begin{bmatrix}\dot{\hat{x}}_{D,i}\\ \dot{\hat{V}}_{nT}\dot{\hat{y}}_{nT,i}\end{bmatrix} = \begin{bmatrix}0 & \dfrac{1}{m_D}\\ 0 & 0\end{bmatrix}\begin{bmatrix}\hat{x}_{D,i}\\ \hat{V}_{nT}\hat{y}_{nT,i}\end{bmatrix} + \begin{bmatrix}\dfrac{-Rx_{D,i}-Dx_{D,i}+\gamma_i\hat{r}_D\varepsilon_D}{m_D}\\ 0\end{bmatrix} - \begin{bmatrix}2\alpha_1\\ \alpha_2^2 m_D\end{bmatrix}[\hat{x}_{D,i}-x_{D,i}] \qquad (15)$$

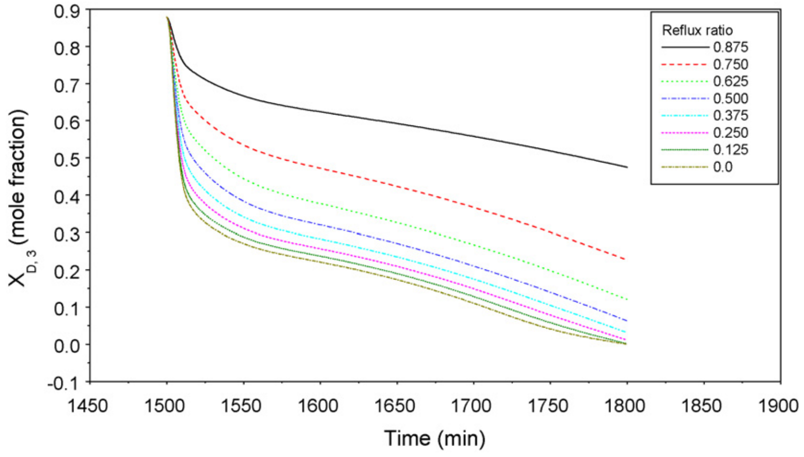

Fig. 4. Sensitivity of the product composition with respect to changes in reflux ratio.

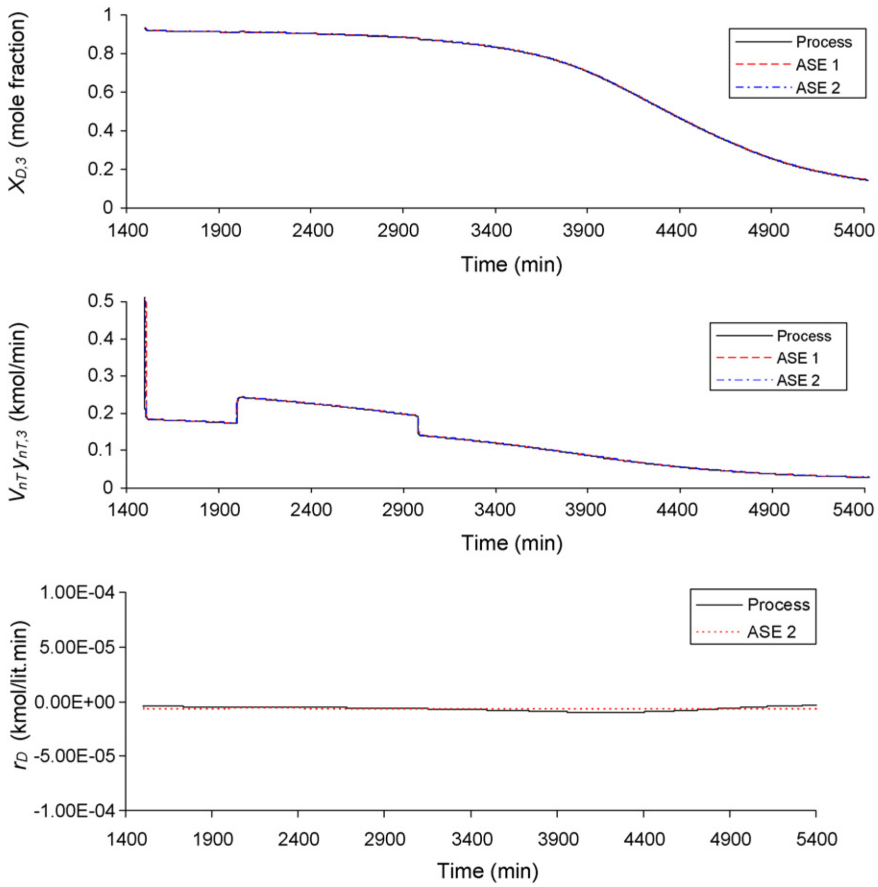

Fig. 5. Comparison of the estimated outputs and process outputs for ethyl acetate with two consecutive step changes in heat input to the reboiler (changed from 3200 to 3520 kJ/min at time = 2000 min and then from 3520 to 3200 kJ/min at time = 3000 min).

Subsystem-2

$$\begin{bmatrix}\dot{\hat{x}}_{D,i}\\ \dot{\hat{r}}_D\end{bmatrix} = \begin{bmatrix}0 & \dfrac{\gamma_i\varepsilon_D}{m_D}\\ 0 & 0\end{bmatrix}\begin{bmatrix}\hat{x}_{D,i}\\ \hat{r}_D\end{bmatrix} + \begin{bmatrix}\dfrac{\hat{V}_{nT}\hat{y}_{nT,i}-Rx_{D,i}-Dx_{D,i}}{m_D}\\ 0\end{bmatrix} - \begin{bmatrix}2\alpha_1\\ \dfrac{\alpha_3^2 m_D}{\gamma_i\varepsilon_D}\end{bmatrix}[\hat{x}_{D,i}-x_{D,i}] \qquad (16)$$

The ASE2 scheme estimates $x_{D,i}$ twice as this state appears in both the subsystems. The value of $V_{nT}y_{nT,i}$ computed in subsystem-1 (Eq. (15)) is used as measured value of that in subsystem-2 (Eq. (16)). The estimation of this parameter ($V_{nT}y_{nT,i}$) may be affected by the measurement noise and if so, the $\hat{x}_{D,i}$ in subsystem-2 may include significant estimation error. Therefore, the value of estimated $x_{D,i}$ ($\hat{x}_{D,i}$) in subsystem-1 has been used to compute the residual and evaluate the ASE2 estimator performance. The value of an additional estimator tuning parameter α_3 is chosen as: 0.055.

4.2. Gain-scheduled proportional integral control system

In a batch distillation column, a low-plant-gain composition space (i.e., the steady state space) changes to a high-plant-gain composition space. This reveals that the control gain should be increased during the batch operation. For this purpose, a gain-scheduled PI law [42] has been designed for the representative process. The GSPI has the following form:

$$R = R_S + K_C(x_{D,i})\left(e + \frac{1}{\tau_i}\int_0^t e\,dt\right) \qquad (17)$$

Here, $x_{D,i}$ is the scheduling variable. The controller gain, K_C, is varied aiming to keep $K_C K_P$ constant, which then keeps the stability margin constant. When the process gain is characterized as a function of the scheduling variable, $K_P(x_{D,i})$, then the controller gain can be scheduled as:

$$K_C(x_{D,i}) = \frac{K_C(x_{D0,i})K_P(x_{D0,i})}{K_P(x_{D,i})} \qquad (18)$$

The gain of the GSPI scheme used has the following forms:

Table 2
Summary of the open-loop estimation results.

Figure	Step change	ISE (ASE1)		ISE (ASE2)		
		$x_{D,3}$	$V_{nT}y_{nT,3}$	$x_{D,3}$	$V_{nT}y_{nT,3}$	r_D
5	Step changes in Q_R	0.0000442	0.0001127	0.0000389	0.000258	0.00001371
6	Step changes in tray efficiency	0.0000439	0.0001113	0.0000369	0.000241	0.00001385
7	Initialization error in $V_{nT}y_{nT,3}$ and r_D	0.0000439	0.0001112	0.0000387	0.000281	0.00001416

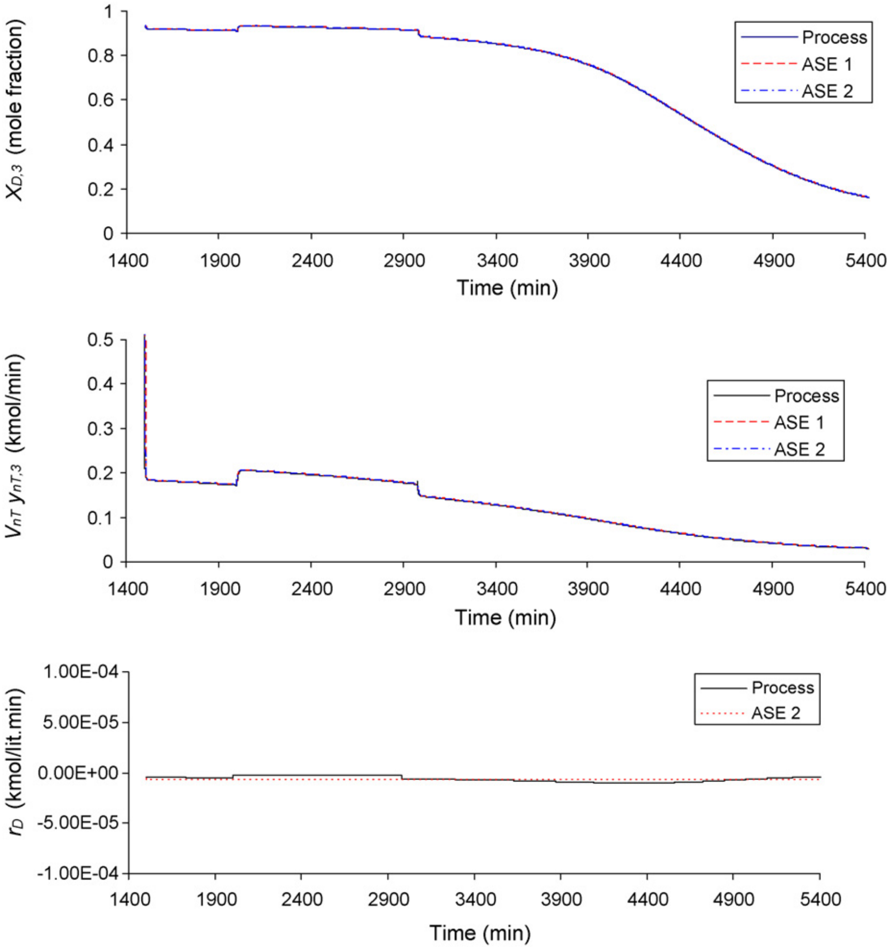

Fig. 6. Comparison of the estimated outputs and process outputs for ethyl acetate with two consecutive step changes in tray efficiency (changed from 0.75 to 0.825 at time = 2000 min and then from 0.825 to 0.75 at time = 3000 min).

(i) when $x_{D,i} > x_{D0,i}$,

$$K_C(x_{D,i}) = K_{C0}\frac{1 - x_{D0,i}}{1 - x_{D,i}} \tag{19}$$

where, $K_P(x_{D,i}) = 1 - x_{D,i}$ and $K_C(x_{D0,i}) = K_{C0}$.

(ii) when $x_{D,i} < x_{D0,i}$

$$K_C(x_{D,i}) = K_{C0} \tag{20}$$

It is worthy to mention that this is a *one-way* approach. Since the process gain increases with lower purity, maintaining a constant controller gain speeds up the response when the distillate is less pure. The tuning of the controller parameters has been performed using the integral square error (ISE) performance criteria and the values of these parameters are obtained as: $K_{C0} = 1.16$ and $\tau_i = 0.15$.

5. Simulation results

Several simulation experiments have been carried out on the reactive batch rectifier in open-loop as well as closed-loop mode to illustrate the developed algorithms. In a standard reactive column, both the reaction and separation take place simultaneously. Among the reactants and product components of the representative system, ethyl acetate has the lowest boiling temperature. So, the ethyl acetate enriched mixture comes out as the distillate product.

In a typical batch distillation operation, first the column may be brought to the steady state by following the total reflux start-up procedure. Then the production phase is begun with switching on the controller as well as the estimator to maintain the specified product purity. In some cases, however, the product is withdrawn as soon as the overhead composition reaches its desired value, without waiting for the steady state to be attained.

At the very beginning of the start-up phase of batch operation, the sample column operates under total reflux condition without having esterification reaction. In such a situation, the batch distillation process, originally a nonreactive ternary (acetic acid/ethanol/water) batch process, reaches at steady state within about 11 min. The next part of the start-up phase runs under complete reflux condition but with having esterification reaction. At the end of start-up phase, the reactive batch column attains another steady state with the ethyl acetate composition of 0.9344. This composition data imposes an upper limit in the achievable product purity under batch operation. The start-up dynamics of the uncontrolled distillate composition, with no reaction in the first part followed by esterification reaction in the last part, are presented in Fig. 3.

It is a well-known fact that in general, the distillation processes are slightly nonlinear in nature. To examine the nonlinearity of the concerned batch reactive distillation, the sensitivity of the product composition has been analyzed in Fig. 4 with respect to changes in reflux ratio. Smooth composition dynamics are observed from the simulation results. It suggests that the process behaves like a linear integrator.

The following discussion is two-fold. In the first part, the tracking performance of the two ASE estimators has been inspected. In the subsequent part, the performance of the proposed adaptive

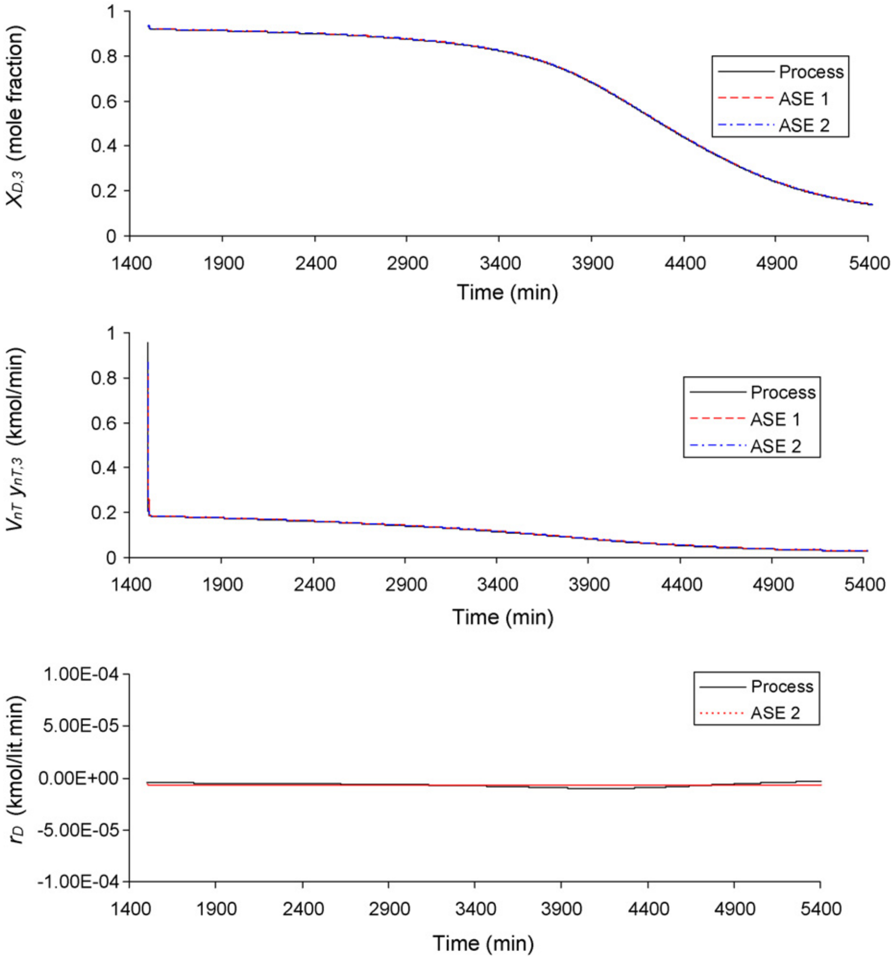

Fig. 7. Comparison of the estimated outputs and process outputs with +10% initialization error in both $V_{nT}y_{nT,3}$ (0.8692 → 0.9561 kmol/min) and r_D (−0.00000417 → −0.00000458 kmol/L min).

controller has been compared with that of the gain-scheduled PI law.

5.1. *Tracking performance of ASE estimators*

5.1.1. *Disturbance in heat input to the reboiler*

Fig. 5 depicts the performance of ASE1 and ASE2 under two consecutive step changes in heat input to the reboiler (step increase: 3200 → 3520 kJ/min at time = 2000 min, and step decrease: 3520 → 3200 kJ/min at time = 3000 min). Despite a large process/predictor mismatch, the numerical results show a satisfactory convergence of the estimated outputs with their true values. Table 2 evaluates the estimation performance in terms of the ISE data.

5.1.2. *Uncertain tray efficiency*

Fig. 6 displays the effect of uncertain tray efficiency (step increase: 0.75 → 0.825 at time = 2000 min, and step decrease: 0.825 → 0.75 at time = 3000 min). Both the ASE schemes provide the estimated outputs that are in good agreement with the actual process outputs. This test shows (Fig. 6 and Table 2) an excellent estimation ability of the developed ASE schemes.

5.1.3. *Initialization error*

The initialization error rejection performance of the ASE estimators is demonstrated in Fig. 7. At the beginning of the production phase (1500 min), the initialization error is

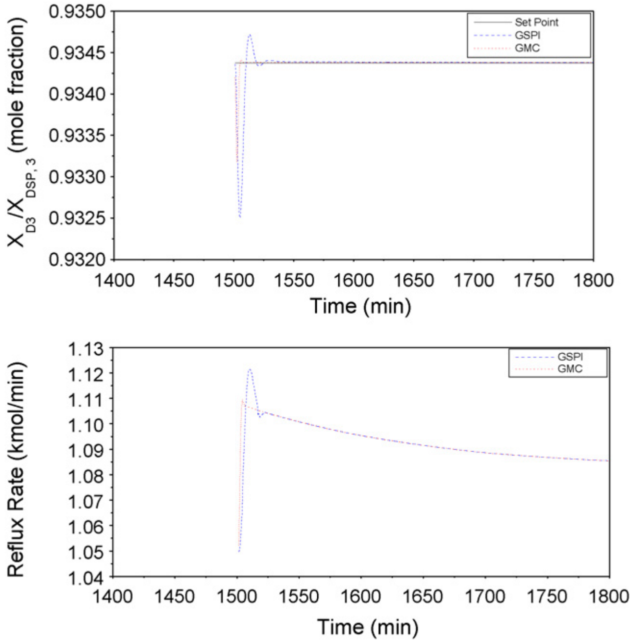

Fig. 8. Comparative performance of the nonlinear adaptive controller and gain-scheduled PI controller for constant composition control ($x_{DSP,3}$ = 0.9344).

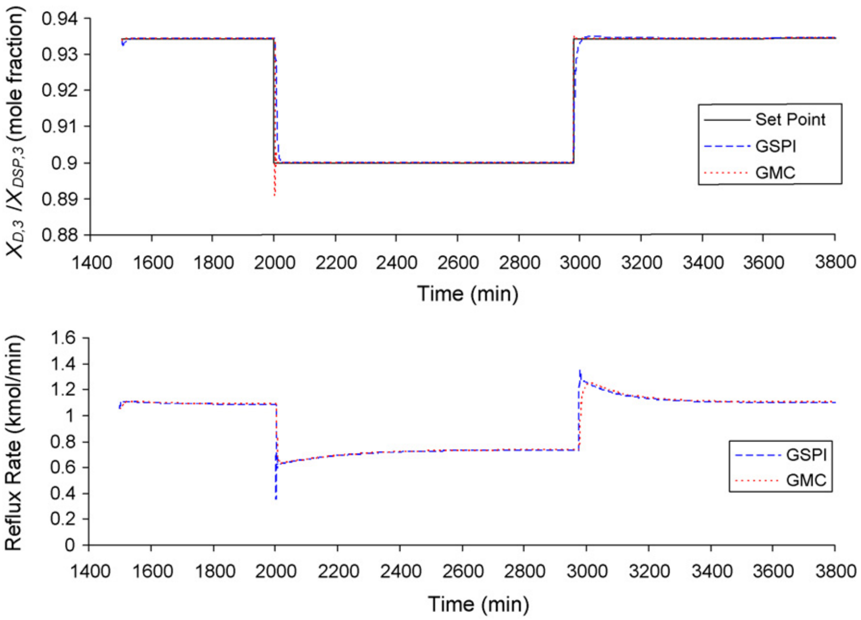

Fig. 9. Comparative servo performance of the nonlinear adaptive controller and gain-scheduled PI controller with two consecutive set point step changes in $x_{D,3}$ (changed from 0.9344 to 0.9 at time = 2000 min and then from 0.9 to 0.9344 at time = 3000 min).

introduced both in $V_{nT}y_{nT,3}$ (0.8692 → 0.9561 kmol/min) and r_D (−0.00000417 → −0.00000458 kmol/L min). Under this situation, the estimation schemes show good convergence ability.

5.2. Comparative closed-loop performance of GMC–ASE and GSPI

A systematic closed-loop performance study is carried out to compare the proposed GMC–ASE1 structure with the GSPI algorithm. In the following, the simulation results of constant composition control, and set point tracking and disturbance rejection performance are presented.

5.2.1. Constant composition control

Fig. 8 illustrates the closed-loop performance of the adaptive nonlinear control law and the GSPI scheme for maintaining the top product composition of the concerned batch reactive rectifier at the value of 0.9344 (reference/steady state composition). The figure also includes the manipulated input profile. Simulation experiment shows that as the product removal starts, the estimator outputs become inaccurate and also the controller responses are aggressive enough. Comparatively, the control action provided by the GSPI is more aggressive than that of the adaptive control system. After about 80 min, the product purity is maintained at its reference value. Table 3 evaluates the comparative performance in terms of the ISE values.

5.2.2. Servo test

Fig. 9 investigates the set point tracking performance of the proposed control strategy. In the present simulation, two subsequent set point step changes in $x_{D,3}$ (step decrease:

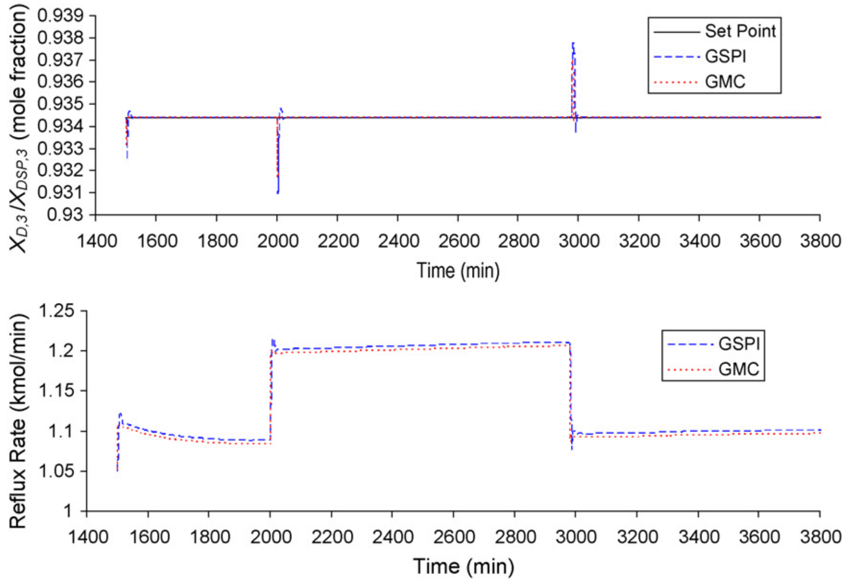

Fig. 10. Comparative regulatory performance of the nonlinear adaptive controller and gain-scheduled PI controller for two consecutive step changes in reboiler heat duty (changed from 3200 to 3520 kJ/min at time = 2000 min and then from 3520 to 3200 kJ/min at time = 3000 min).

Table 3
Summary of the closed-loop control results.

Figure	Step change	ISE (adaptive)	ISE (GSPI)
8	Constant composition (0.9344) control	0.0000022574	0.000013578
9	Servo test: step changes in $x_{D,3}$	0.00121648	0.00986794
10	Regulatory test: step changes in Q_R	0.00002173	0.00010325

0.9344 → 0.9 at time = 2000 min, and step increase: 0.9 → 0.9344 at time = 3000 min) have been introduced. The results show that the proposed adaptive controller performs better than the GSPI control scheme. Table 3 confirms the superiority of the GMC–ASE structure over the GSPI.

5.2.3. *Regulatory test*

A comparative disturbance rejection performance is presented in Fig. 10 considering two consecutive step changes in reboiler heat duty (step increase: 3200 → 3520 kJ/min at time = 2000 min, and step decrease: 3520 → 3200 kJ/min at time = 3000 min). Despite a large unmodeled dynamics involved in ASE estimator of the GMC–ASE structure, it is observed from Fig. 10 that the adaptive control law provides better regulatory performance than the GSPI controller. Table 3 supports this observation.

6. Conclusions

The present work has proposed an adaptive GMC–ASE control system for a reactive batch distillation column that produces ethyl acetate by the esterification of ethanol with acetic acid. The control system comprises of a nonlinear generic model controller and a closed-loop adaptive state estimator.

Structural and parametric discrepancies are considered between the actual process and the predictor model in order to provide a realistic test scenario for the proposed strategy. Despite the structural perturbation, both the estimation schemes give sufficiently fast convergence in presence of disturbance and parametric uncertainty.

The GMC–ASE control law provides tight composition control throughout the batch operation. Better set point tracking and disturbance rejection performance is achieved by the nonlinear adaptive controller compared to the GSPI scheme. The simple design, easy tuning and good performance make the adaptive controller attractive for online use.

Appendix A

The model structure of the sample batch reactive rectifier has been developed based on the following assumptions:

- Negligible tray vapour holdups
- Variable liquid holdup in each tray
- Perfect mixing and equilibrium on all trays
- No chemical reactions in the vapour-phase
- Reactions occurred on the trays, and in the condenser and reboiler
- Fast energy dynamics
- Constant operating pressure (atmospheric) and tray efficiencies (Murphree vapour-phase efficiency = 75%)
- Total condensation with no subcooling
- Raoult's law for the vapour–liquid equilibrium
- No azeotropes formation
- Nonlinear Francis weir formula [43] for liquid hydraulics calculations
- Constant liquid holdup in the reflux drum (perfectly controlled by a conventional proportional (P-only) controller with a proportional gain of −0.01)

To perform the simulation experiments, the process is modelled using a detailed tray-to-tray model. The model structure of a reactive batch distillation column is summarized below.

A.1. *Reboiler equations*

Total mole balance:

$$\dot{m}_B = L_1 - V_B + \sum_{i=1}^{C} \gamma_i r_B \varepsilon_B \qquad (A1)$$

Component mole balance:

$$\dot{m}_B \dot{x}_{B,i} = L_1 x_{1,i} - V_B y_{B,i} + \gamma_i r_B \varepsilon_B \qquad (A2)$$

Energy balance:

$$\dot{m}_B \dot{H}_B^L = L_1 H_1^L - V_B H_B^V + r_B \varepsilon_B H_B^r + Q_R \qquad (A3)$$

Equilibrium:

$$y_{B,i} = K_{B,i} x_{B,i} \qquad (A4)$$

A.2. *Condenser equations*

Total mole balance:

$$\dot{m}_D = V_{nT} - (R + D) + \sum_{i=1}^{C} \gamma_i r_D \varepsilon_D \qquad (A5)$$

Component mole balance:

$$\dot{m}_D \dot{x}_{D,i} = V_{nT} y_{nT,i} - (R + D) x_{D,i} + \gamma_i r_D \varepsilon_D \qquad (A6)$$

Energy balance:

$$\dot{m}_D \dot{H}_D^L = V_{nT} H_{nT}^V - (R + D) H_D^L + r_D \varepsilon_D H_D^r - Q_C \qquad (A7)$$

Equilibrium:

$$y_{D,i} = K_{D,i} x_{D,i} \qquad (A8)$$

A.3. *Stage equations*

Total mole balance:

$$\dot{m}_n = L_{n+1} + V_{n-1} - L_n - V_n + \sum_{i=1}^{C} \gamma_i r_n \varepsilon_n \qquad (A9)$$

Component mole balance:

$$\dot{m}_n \dot{x}_{n,i} = L_{n+1} x_{n+1,i} + V_{n-1} y_{n-1,i} - L_n x_{n,i} - V_n y_{n,i} + \gamma_i r_n \varepsilon_n \qquad (A10)$$

Energy balance:

$$\dot{m}_n \dot{H}_n^L = L_{n+1} H_{n+1}^L + V_{n-1} H_{n-1}^V - L_n H_n^L - V_n H_n^V + r_n \varepsilon_n H_n^r \qquad (A11)$$

Equilibrium:

$$y_{n,i} = K_{n,i} x_{n,i} \qquad (A12)$$

In the preceding process model, the dot symbol (.) is used to represent the time derivative. The time derivative of the multiplication of two variables, say m and x, is denoted here by $\dot{m}\dot{x}$ (=$d(mx)/dt$). In the simulation, algebraic form of equations [44] has been used to compute the vapour and liquid enthalpies. Heat of formation is considered while calculating the enthalpies of streams by means of which the heat of reaction term can be removed from the energy balance equation.

In this work, the simulated model has been referred to as "the process". At the beginning of the batch operation, it is assumed that the reboiler, all the trays, and the reflux drum are filled with the liquid feed. As suggested by Mujtaba and Macchietto [40], the 4% of the total feed charge is used as total column holdup. Half of this holdup is taken as reflux accumulator holdup and the rest is equally divided for the tray holdups.

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