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Dynamic composition estimation for a ternary batch distillation

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ABSTRACT

A novel Kalman estimator has been proposed to provide the estimates of dynamic composition in a ternary batch distillation process operated in an optimal-reflux policy. The estimator is formulated based on a sequence of reduced-order process models representing a whole batch behavior. Therefore, the full-order models are first developed around different pseudo-steady-state operating conditions along batch optimal profiles. Then they reduce their orders to achieve all state observability and controllability by a balanced truncation method. In the estimator scheme, the reduced models as well as relevant covariance matrices of process noise are pre-scheduled and switched according to any desired periods. Four important issues have been studied including selection of a sensor frequency, effects of an integrating step size, a state initialization and a measurement noise. The performances of the reduced estimator have been investigated and compared with those of a conventional nonlinear estimator. Simulation results have demonstrated that the performances of the novel linear estimator are reasonably good and almost identical to the nonlinear estimator in all cases, though the linear estimator performs rather sensitively to the effect of high measurement noise. Nevertheless, it has been found to be applicable to implement in real plants with much lower computation effort, easier state initialization and unrequired a priori knowledge of thermodynamics.

1. Introduction

Batch distillation is an important unit operation widely used in fine chemistry, pharmaceutical, biochemical and food industries to process small amounts of materials with high added value. The main reason is its operational flexibility that a single column can separate all components of a multi-component mixture into several products within a single operation. So as to meet product specification, the batch column needs to be operated as precisely as possible. If instant compositions are known, an automatic closed-loop control scheme can be implemented correctly to drive the process to the desired operating strategy. An inferential composition estimator is then introduced to provide estimates of the composition concentrations based on available temperature measurements. The use of the estimator has long been suggested to assist monitoring and control of a continuous distillation (Yang and Lee, 1997; Zhang, 2001; Kano et al., 2003). Conversely to the batch column, the issue has received little attention.

In the area of batch distillation, most researches have focused on a development of the composition estimator based on a nonlinear fundamental model. An Extended Luenberger Observer (ELO) was primarily applied to a multi-component batch system through the use of the tray temperature measurements (Quintero-Marmol et al., 1991; Luyben, 1992). As the observer was based on a deterministic model and its gains were obtained in off-line fashion, its performance was degraded rapidly when the measurements were affected by noise. Therefore, the use of a stochastic estimator such as a Kalman Filter (KF) was recommended if large amount of noise is expected (Barolo and Berto, 1998). Moreover, the ELO accuracy was likely to degrade if tray hydraulic was taken into account, and increasing number of trays makes the ELO harder to tune. Afterwards, a discrete Extended Kalman Filter (EKF) for the conventional batch distillation was developed to handle the effect of noise by Oisiovici and Cruz (2000). For the reason that its gains were updated online, it could manage to incorporate the effect of noise. Recently, Venkateswarlu et al. (2001, 2006) have applied the EKF scheme for the composition estimation in a batch reactive distillation. Even though the EKF has been proved in literatures to be much more robust to mismatch and noise than the ELO, it is rather difficult to initialize all states and requires considerable computational effort for online use. Furthermore, its performance heavily depends on the thermodynamics modeling of vapor–liquid equilibria.

Alternatively, this work develops a novel linear version of the KF for the conventional ternary batch column to retrieve the distillate and reboiler composition profiles from the temperature measurement information. An idea of using multiple local models

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sequentially is applied for the estimator design. The column is designed to operate in an optimal reflux policy where its dynamic changes rapidly introducing an estimation difficulty of the composition profiles. In most cases the full-order equations contain additional unobservable and/or uncontrollable states. Therefore, the models reduce their orders individually using a balanced truncation method to attain only observable and controllable state contributions. The organization of the paper is as follows. A process description and a determination of the optimum reflux policy are presented in Section 2. Background and implementation of the EKF and of the novel KF are discussed briefly in Sections 3 and 4, while issues concerning the development of a composition prediction model is introduced in Section 5. The performances of both the estimators are investigated in Section 6 and the conclusion is presented in Section 7.

2. A ternary batch distillation

In a conventional batch distillation as shown in Fig. 1, a liquid mixture is charged into a vessel and heat is added to produce vapor fed into a rectifying column. A concentration of the lightest component increases in the upper trays sequentially in the column and a concentration of a subsequent heavy component increases in a still pot. As the concentration of the lightest component in the distillate reaches its specified purity level or the unit in total reflux operation is taken to a steady state, the distillate product withdrawal begins.

2.1. Process description

To develop mathematical models of a ternary batch distillation, constant volume holdup (CVH) for all trays is assumed. The assumption of CVH is reasonably valid because after the total reflux is run, the volume holdup of each tray is relatively negligible in comparison with the volume of the reboiler. Therefore, the volume holdup is rarely changed. Then, the equations describing the process are given below More detailed description of the operation and modeling of

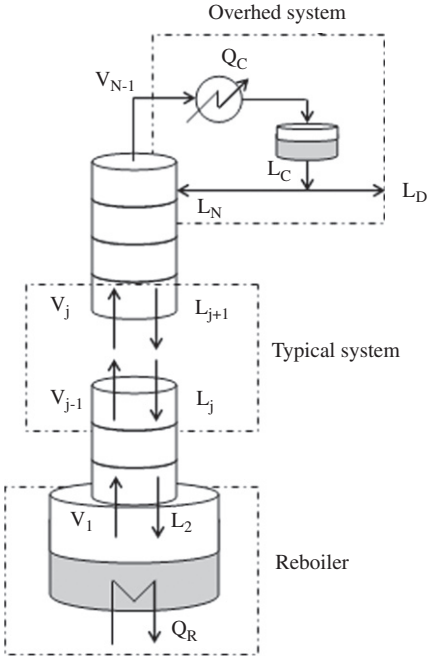


Fig. 1. Schematic representation of a conventional column.

Table 1
Specification of a ternary batch column

Column specification	
No. of ideal separation stages (including a reboiler and a total condenser)	=7
Total fresh feed, B_0, kmol	=2
Component	=⟨acetone, toluene, phenol⟩
Feed composition, x_{B_0}, mole fraction	=[0.4, 0.4, 0.2]
Column volume, liter (at $T = 352.87$ K):	
Condenser	=3.7551
Internal plates	=0.5364
Reboiler	=180.246
Column pressure, mmHg	=760
Heat supplied in reboiler, J/h	$=5 \times 10^7$

the batch column are referred to (Distefano, 1968; Mujtaba, 2004)

$$\frac{dx_{1i}}{dt} = \frac{L_2}{H_1}(x_{2,i} - x_{1i}) - \frac{V_1}{H_1}(y_{1i} - x_{1i}) \tag{1}$$

$$V_1 = \frac{1}{(h_1^v - h_1^l)}(Q_R + L_2(h_2^l - h_1^l) - H_1\delta h_1^l) \tag{2}$$

$$\frac{dx_{ji}}{dt} = \frac{L_{j+1}}{H_j}(x_{j+1,i} - x_{ji}) + \frac{V_{j-1}}{H_j}(y_{j-1,i} - x_{ji}) - \frac{V_j}{H_j}(y_{ji} - x_{ji}) \tag{3}$$

$$L_j = L_{j+1} + V_{j-1} - V_j - \delta H_j \tag{4}$$

$$V_j = \frac{1}{(h_j^v - h_j^l)}(L_{j+1}(h_{j+1}^l - h_j^L) + V_{j-1}(h_{j-1}^v - h_j^l) - H_j\delta h_j^l) \tag{5}$$

$$\frac{dx_{Ni}}{dt} = \frac{V_{N-1}}{H_N}(y_{N-1i} - x_{Ni}) \tag{6}$$

$$L_C = V_{N-1} - \delta H_N \tag{7}$$

$$Q_C = V_{N-1}(h_{N-1}^v - h_N^l) - H_N\delta h_N^l \tag{8}$$

where $L_N = rL_C$. Change rates of molar holdup and liquid enthalpy are approximated by using an Euler integrating approach, i.e.

$$\delta H = \frac{dH}{dt} = \frac{H_k - H_{k-1}}{dt}$$

where k is the current iteration. Reboiler holdup at any time is calculated from the following algebraic combination:

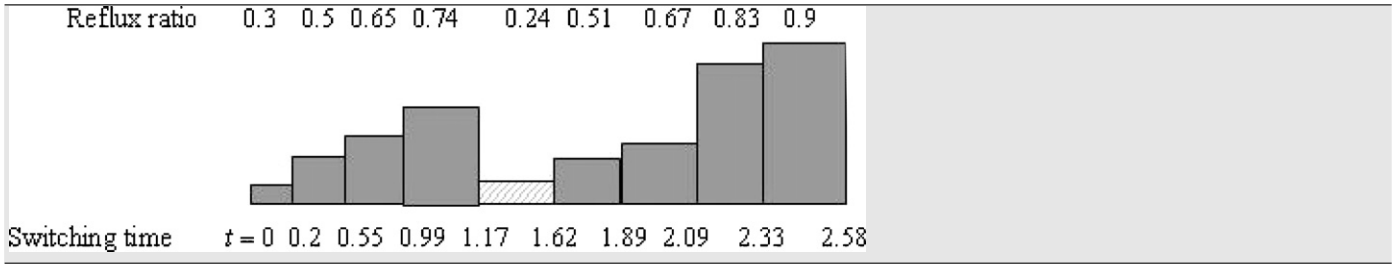
$$H_{1,k} = B_0 - \left(\sum_{j=2}^{N} H_{j,k}\right) - H_{a,k} \tag{9}$$

Antoine's equations are used in a bubble-point calculation, and both liquid and vapor enthalpies are obtained from experimental correlations (Holland, 1981; Reid and Sherwood, 2000). The variation of liquid density is described by using a modified Rackett equation. Column specification used in this study is given in Table 1.

2.2. Optimal reflux policy

In this work, optimal reflux profiles are prior determined by minimizing a final batch time subject to the process Eqs. (1)–(9) and specified product amounts and purities. In this case, the purities of acetone, toluene and phenol are required to be greater than 0.98, 0.98 and 0.995 mole fractions, respectively, as well as the amounts of the products 0.72, 0.36 and 0.34 kmols, respectively. So to solve the dynamic optimization problem, the reflux variables are parameterized into a finite set in which a piecewise constant function is utilized. It is assumed that the operations of each main-cut and off-cut are divided into four and one intervals, respectively, resulting in

Table 2
Optimal results for a ternary batch distillation



20 control variables including 10 reflux variables and 10 switching times. The obtained optimal results given in Table 2 show that the desired residue product can be achieved by neglecting the second off-cut operation. In this case, the optimal batch time is 2.58 h with the first off-cut beginning to collect at time 1.17 h and stopping at 1.62 h.

3. Conventional nonlinear estimator

3.1. An extended Kalman filter (EKF)

A nonlinear process can be described by following differential and measurement equations:

$$\dot{x} = f(x, u) + w$$

$$y = h(x) + v \tag{10}$$

where w and v are vectors of process and measurement noises, respectively, with covariance Q and R, respectively. Corrected estimates are computed as a linear combination of a priori estimates and a weighted difference between actual and predicted measurements:

$$\tilde{x}_{k|k} = \hat{x}_{k|k-1} + K_{\text{est},k}(y_k - h(\tilde{x}_{k|k-1})) \tag{11}$$

where $K_{\text{est},k} = \Sigma_{k|k-1} H_k^{\mathrm{T}} (H_k \Sigma_{k|k-1} H_k^{\mathrm{T}} + R)^{-1}$ is an estimator gain and $H_k = (\partial h(x)/\partial x)|_{\hat{x}_{k|k-1}}$. Corresponding to a state covariance,

$$\Sigma_{k|k} = \Sigma_{k|k-1} - K_{\text{est},k} H_k \Sigma_{k|k-1} \tag{12}$$

For a prediction step, the estimates for the next time step are predicted based on the current estimates in which the discrete prediction equations are employed:

$$\tilde{x}_{k+1|k} = \bar{f}(\tilde{x}_{k|k}, u_k) \tag{13}$$

The concerning covariance matrix can be rewritten as

$$\Sigma_{k+1|k} = F_k \Sigma_{k|k} F_k^{\mathrm{T}} + Q \tag{14}$$

where

$$F_k = \left(\frac{\partial \bar{f}(x, u)}{\partial x} \right) \Bigg|_{\hat{x}_{k|k}, u_k}$$

3.2. Implementation of EKF

As the nonlinear estimator-based rigorous mathematical model of an actual plant is rather complex, a simplified model integrated with a bubble-point calculation is easier to be employed in practice. The simplified equations are given by

$$\frac{\mathrm{d}x_{1i}}{\mathrm{d}t} = \frac{rV}{H_1}(x_{2i} - x_{1i}) - \frac{V}{H_1}(y_{1i} - x_{1i}) \tag{15}$$

$$\frac{\mathrm{d}x_{ji}}{\mathrm{d}t} = \frac{V}{H_j}(y_{j-1,i} - y_{ji}) + \frac{rV}{H_j}(x_{j+1,i} - x_{ji}) \tag{16}$$

$$\frac{\mathrm{d}x_{Ni}}{\mathrm{d}t} = \frac{V}{H_N}(y_{N-1,i} - x_{Ni}) \tag{17}$$

At each integration step in an EKF scheme, a reboiler holdup prediction is obtained as

$$H_{1,k} = B_0 - (N-2) \times H_j - H_N - H_{a,k}$$

where

$$H_{a,k} = H_{a,k-1} + \Delta t \times [(1-r)V]$$

In this case, a state vector is $[x_{11}, x_{21}, \ldots, x_{N1}, x_{12}, x_{22}, \ldots, x_{N2}]^{\mathrm{T}}$ in which only the first two components are considered. The heaviest component can be obtained by subtracting the summation of the first two components from one. The measurement equations are derived from Antoine's equations. From Eqs. (15)–(17), the knowledge of H_j, H_N and V are acquired. In the work of Oisiovici and Cruz (2000), the instant vapor flow rate is estimated by the knowledge of vaporization heat and heating power. Nevertheless, the exact calculation of the heat of vaporization is difficult; hence, the assumption of the constant vapor load along the batch is made here. The constant values of the parameters H_j, H_N and V are obtained in an optimal manner as 0.0052, 0.0427 and 1.4195 kmol/h, respectively.

4. A novel estimator scheme

An application of an EKF estimator to a batch distillation for estimating column compositions has not much been reported in literatures, even though the EKF is proved to be robust to mismatch and noise. The main reasons are that it requires considerable computational effort for online use and a priori thermodynamic knowledge which is rarely known in reality. Moreover, it is difficult to initialize all states of the column perfectly. A novel linear version of a KF estimator is then proposed in this section to overcome those problems. In a continuous process, an accurate linear model can be easily obtained. Conversely, a batch process description using a single local model is rarely possible because of non-stationary and time-varying behavior. On the other hand, the batch representation can be achieved using a sequence of the local models as shown in Fig. 2. This modeling strategy is motivated by the fact that the batch system goes through a series of phases with substantially different characterization. The individual model is employed for an output prediction within a particular duration. The models are developed around different pseudo-steady-state operations along the reference batch profiles.

4.1. A novel KF approach

Once measurements are available, the model states and outputs are updated and predicted for the next step by using the

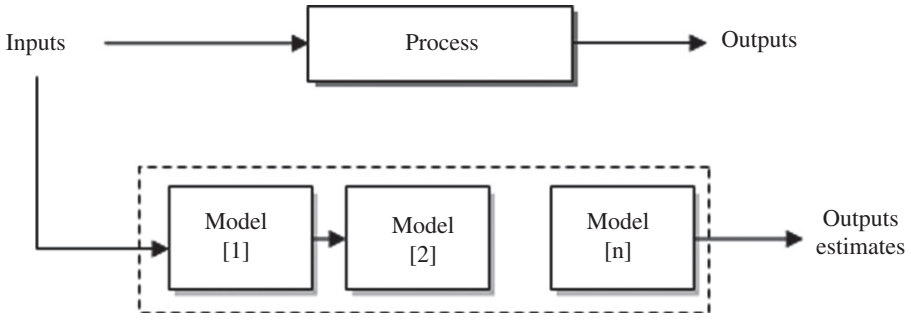


Fig. 2. Representation of a batch column using a sequence of multiple models.

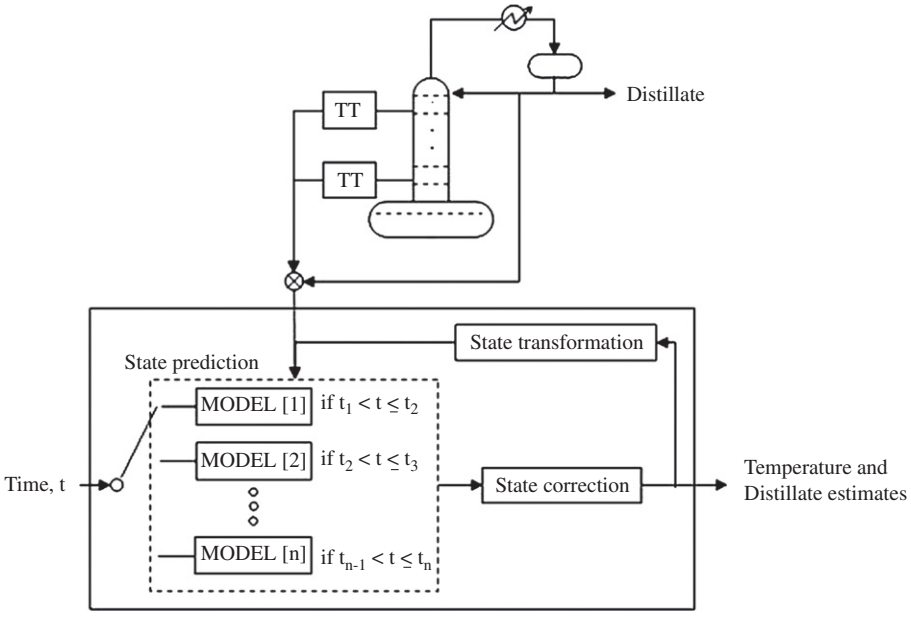


Fig. 3. Estimation scheme of KF-based multiple models.

corresponding model equations. An estimation scheme of the novel KF-based multiple models is shown in Fig. 3. As in most cases the original full states contain additional unobservable and/or uncontrollable states; the obtained full models should reduce their orders separately to attain only observable state contributions by using a model reduction approach. Since ranks of observability matrices vary along the batch, the reduced models may have a different number of states. At a model connection, a state covariance matrix Σ is transformed by multiplying matrix K_j for an estimation consistency as follows:

$$\Sigma_{k|k,j+1} = K_j \Sigma_{k|k,j} K_j^{\mathrm{T}} \tag{18}$$

Although the models are in different state domains and may obtain different model orders, process inputs and outputs are identical,

$$y = C_j x_j = C_{j+1} x_{j+1} \tag{19}$$

The transform matrix K_j can be simply derived from the above equation,

$$K_j = (C_{j+1}^{\mathrm{T}} C_{j+1})^{-1} C_{j+1}^{\mathrm{T}} C_j, \tag{20}$$

where

$$x_{j+1} = K_j \cdot x_j$$

It can be seen that matrix K_j is only dependent on the measurement of matrices C of the two considered models (j) and ($j+1$); in other words it is independent of instant time. Table 3 summarizes the estimation approach of the KF-based multiple models. It can be seen that the conventional KF with a single model can be executed by discarding steps 1 and 2.

Table 3
An approach of KF estimator-based multiple models

STEP 0:	$t, y_k, \hat{x}_k, \mathrm{d}t$
STEP 1:	Current model specification, j_k (at time t)
	$\Theta_{j,k} \rightarrow \{A, B, C, D\}$ in which $j = \begin{cases} 1 & t_0 < t \leqslant t_1 \\ 2 & t_1 < t \leqslant t_2 \\ . & . \\ n & t_{n-1} < t \leqslant t_f \end{cases}$
STEP 2:	State and covariance transformation,
	IF $j_k \neq j_{k-1}$ THEN
	$\hat{x}_{k,j} = K_{j-1} \cdot \hat{x}_{k,j-1}$ and $\Sigma_{k,j} = K_{j-1} \Sigma_{k,j-1} K_{j-1}^T$
	ELSE GO TO STEP 3 END
STEP 3:	Correction step:
	$\hat{x}_{k\|k} = \hat{x}_{k\|k-1} + K_{\mathrm{est}}(y_k - C\hat{x}_{k\|k-1})$
	$\Sigma_{k\|k} = \Sigma_{k\|k-1} - K_{\mathrm{est}} C \Sigma_{k\|k-1}$
	where, $K_{\mathrm{est}} = \Sigma_{k\|k-1} C^{\mathrm{T}} (C \Sigma_{k\|k-1} C^{\mathrm{T}} + R)^{-1}$
STEP 4:	Prediction step:
	$\hat{x}_{k+1\|k} = A\hat{x}_{k\|k} + Bu_k$
	$\Sigma_{k+1\|k} = A \Sigma_{k\|k} A^{\mathrm{T}} + Q$
STEP 5:	IF $t < t_f$ THEN
	$k = k + 1$
	GO TO STEP 0
	ELSE STOP END

4.2. Implementation of a novel estimator

By applying a local linearization to nonlinear model equations, a first-order Taylor approximation is employed in which for a continuous process the steady term is zero at the steady-state operating condition. However, the steady term does not exist for a batch system because there is no such steady-state operating point. An augmented state vector including a differentiated state ($\Delta x_{r,k}=x_{r,k}-x_{r,k-1}$) vector and the measurable outputs is introduced instead of using the model states solely to eliminate the constant term,

$$\begin{vmatrix} \Delta x_{r,k+1} \\ C_{Tr}\cdot x_{r,k+1} \end{vmatrix} = \begin{vmatrix} \phi & 0 \\ C_{Tr}\cdot\phi & I \end{vmatrix} \cdot \begin{vmatrix} \Delta x_{r,k} \\ C_{Tr}\cdot x_{r,k} \end{vmatrix} + \begin{vmatrix} \gamma \\ C_{Tr}\cdot\gamma \end{vmatrix} \cdot |\Delta u_k|$$
$$y_{T,k} = |0 \;\; I| \cdot \begin{vmatrix} \Delta x_{r,k} \\ C_{Tr}\cdot x_{r,k} \end{vmatrix} \tag{21}$$

where $\phi=[I+\Delta t\cdot A_r]$, $\gamma=[\Delta t\cdot B_r]$ and Δt is an integrating interval. If the current augmented states are known, the unmeasurable outputs can be calculated from the following equation:

$$y_{x,k} = |C_{xr} \;\; 0| \cdot \begin{vmatrix} \Delta x_{r,k} \\ C_{Tr}\cdot x_{r,k} \end{vmatrix} + y_{x,k-1} \tag{22}$$

The main advantages of using the augmented states are that the constant term which results from the linearization can be discarded. In addition, the differentiated states can be initialized easily with the values of zero. It is noted that this work develops the state-space models based on the first-principle equations; alternatively, one can obtain the system matrices through experimental information by using a subspace state-space identification method (Favoree et al., 2000; Jimenez et al., 2002; Andrew and Jay, 2003).

5. Composition prediction model

5.1. A model reduction approach

In most cases, a full-local model contains additional unobservable and/or uncontrollable states. However, only observable and controllable states are needed for monitoring and control. A balanced truncation method is then applied to attain only the observable and controllable contributions. Table 4 summarizes the approach of the reduction method for an unstable system. For more details of the approach refer to Nering (1963), Skogestad and Postlethwaite (1996) and Zhou and Doyle (1998). Because the reduction method cannot be applied directly to the unstable process, the system matrix A of the original realization $\Theta\rightarrow\{A,B,C,D\}$ should be firstly diagonalized for simply identifying stable and unstable parts of the system. It is noted that the elements in the main diagonal of A_d are the eigenvalues of A. The stable realization is balanced subsequently that both observability and controllability gramians are equal and diagonal. The less observable and controllable states of the balanced realization are further truncated. A measure of the accuracy of the method is an error in H_∞ norm of the approximation, and it should satisfy the inequality equation as shown in step 4. In this work, the maximum value of the error has been arbitrarily chosen as 0.0001. In the last step, the reduced stable and unstable parts are composed together to preserve the main characteristic of the process.

Table 4
A balanced truncation approach

STEP 0:	Model realization: $\Theta\rightarrow\{A,B,C,D\}$, x
STEP 1:	System diagonalization [MATLAB command: *strans*]: $\Theta_d\rightarrow\{A_d,B_d,C_d,D_d\}$, where, $x_d=v^{-1}x$, $A_d=v^{-1}Av$, $B_d=v^{-1}B$, $C_d=Cv$ and $D_d=D$
STEP 2:	Stable and unstable parts decomposition: $\Theta_s\rightarrow\{A_s,B_s,C_s,D_s\}$ where A_s contains only negative eigenvalues $\Theta_u\rightarrow\{A_u,B_u,C_u,D_u\}$ where A_u contains only positive eigenvalues
STEP 3:	Balanced realization [MATLAB command: *balreal*]: $\Theta_b\rightarrow\{A_b,B_b,C_b,D_b\}$, where, $x_b=Sx_s$, $A_b=SA_sS^{-1}$, $B_b=SB_s$, $C_b=C_sS^{-1}$ and $D_b=D_s$
STEP 4:	Truncation approach [MATLAB command: *modred*(*mod*, []`*del*')]: $\sigma_{nr+1}\leqslant\|G-G_{rs}\|_\infty\leqslant 2\sum_{i=nr+1}^{nx}\sigma_i$ where, $G$ and $G_{rs}$ are transfer functions of full and reduced-order model. Let $nr=nx$ WHILE $2\sum_{i=nr+1}^{nx}\sigma_i>0.0001$ $nr=nr-1$; modred(mod, [$nr+1:nx$], `del'); END $\Theta_{rs}\rightarrow\{A_{rs},B_{rs},C_{rs},D_{rs}\}$
STEP: 5	Reduced and unstable parts combination: $\Theta_r=\Theta_{rs}+\Theta_u=\left[\begin{array}{cc\|c} A_{rs} & 0 & B_{rs} \\ 0 & A_u & B_u \\ \hline C_{rs} & C_u & D_{rs}+D_u \end{array}\right]$

The original measurement equation considering only the measurable outputs is

$$y_T = C_T\cdot x \tag{23}$$

where x is a composition vector $[x_{11},x_{21},\ldots,x_{N1},x_{12},x_{22},\ldots,x_{N2}]^{\mathrm{T}}$. By applying Table 4 the output equation in the reduced-state domain, x_r can be obtained as

$$y_T = [C_{Tb}|_{ny\times nr} \;\; C_{Tu}]\cdot x_r = C_{Tr}\cdot x_r \tag{24}$$

where $C_{Tu}=C_{Td}^{+}$ and $C_{Tb}=C_{Td}^{-}S^{-1}$ in which C_{Td}^{+}, C_{Td}^{-} are the matrix $C_{Td}(C_{Td}=C_Tv)$ corresponding to positive and negative eigenvalues, respectively, and $C_{Tb}|_{ny\times nr}$ is the matrix C_{Tb} that the last $(nr+1)$ to nx columns are truncated. From the full-order model, the distillate compositions can be monitored as

$$\begin{bmatrix} x_{N1} \\ x_{N2} \\ x_{11} \\ x_{12} \end{bmatrix} = \begin{bmatrix} 0 & . & 1 & 0 & . & 0 \\ 0 & . & 0 & 0 & . & 1 \\ 1 & . & 0 & 0 & . & 0 \\ 0 & . & 0 & 1 & . & 0 \end{bmatrix} \cdot x$$
$$y_x = C_x\cdot x \tag{25}$$

where the compositions of a distillate and a reboiler are monitored. Similarly, a prediction equation of the compositions in x_r domain is obtained as follows:

$$y_x = C_{xr}\cdot x_r \tag{26}$$

where $C_{xr}=[C_{xb}|_{4\times nr} \;\; C_{xu}]$, $C_{xb}=C_{xd}^{-}S^{-1}$ and $C_{xu}=C_{xd}^{+}\cdot C_{xd}^{+}$, C_{xd}^{-} are the matrix $C_{xd}(C_{xd}=C_xv)$ corresponding to unstable and stable eigenvalues, respectively, and $C_{xb}|_{4\times nr}$ is the matrix C_{xb} where only the first nr columns are considered. The system equations considering both the measurable and unmeasurable outputs can be rewritten as

$$\dot{x}_r = A_r\cdot x_r + B_r\cdot u$$
$$\begin{bmatrix} y_T \\ y_x \end{bmatrix} = \begin{bmatrix} C_{Tr} \\ C_{xr} \end{bmatrix}\cdot x_r \tag{27}$$

In the estimation scheme, the reduced-state estimates are updated at each iteration by using available information of actual and predicted

5.2. A prediction model for a composition estimation

For a batch distillation, the process outputs consist of measurable tray temperatures and unmeasurable product compositions. It is noted that the reduced models developed above consider only the measurable outputs. In spite of this a monitoring of the instant product compositions is also required for a precise implementation of a control strategy. In this sub-section, a prediction model for dynamic composition estimation is derived in a reduced-state domain.

temperature measurements. Then, the un-measurable product compositions are estimated using the current estimates of the reduced states. The estimates for the next step are predicted by using Eq. (27).

6. Simulation results

Inferential composition estimation for a ternary batch column operated in an optimal operation is studied here. Optimal profiles are pre-determined by minimizing a total batch time to yield desired product quantity and purity. The optimal solution is obtained with two main-cuts and one off-cut. In this system, acetone and toluene are separated as distillate products and phenol is separated as a residual product in a still pot. For solving the rigorous model (Eqs. (1)–(9)), backward differentiation formula or Gear's type method, an implicit numerical method, is employed. An approximation of the differential equations used in the estimators is achieved by using an Euler integration method. All simulations studied are carried out on Window XP 2002 (Pentium M 1500 MHz) by using MATLAB program version 6.5.

6.1. Multiple model development

As mentioned earlier, it is rarely possible to predict a whole batch behavior by a single linear model. Therefore, a set of models are developed based on batch trajectory and used sequentially along a batch operation. Here, it has been found that as instant distillate compositions remarkably change every 5 min during the operation period, the novel estimator is activated 5 min in all cases. Consequentially, a series of 35 models are developed and employed to represent a whole batch operation involving 16 models for the first main-cut, 6 models for off-cut and 13 models for the second main-cut.

The 35 models developed contain 14 full states (no. of total plates 7×2 components), including additional unobservable states. For good monitoring, the models further reduce their order individually using a balanced truncation method. It is assumed that all tray temperatures are measurable (six sensors) in all cases. Fig. 4a shows error in the H_∞ norm as well as lower and upper bounds calculated from the inequality equation as given in Table 4 (step 4). The reduced orders are plotted with time as shown in Fig. 4b. It is noted that by applying model reduction the original full states can be computed as a linear combination of the new reduced states. In the off-cut operation, the highest reduced orders are obtained because composition changes of both the components are significant. Afterwards, the model order decreases continuously in the production of toluene. Since the acetone amount in the column is completely exhausted and removed from the column, only seven new states are required for the last model.

As the batch process is operated in an optimal reflux policy, the dynamic behavior of the system changes correspondingly during the batch, leading to difficulty in the estimation/control. For the reason that the reduced models are developed separately and the process is highly nonlinear, the developed models may give poor dynamics response. It is a fact that estimates of an estimator are poor for the whole batch with the use of a fixed value of process covariance. Therefore, 35 matrices Q are defined and scheduled according to the corresponding model equations. However, the diagonal elements of the matrices R and Σ_0 are constant at 10 and 10^{-5}, respectively. For the EKF estimator, the diagonal elements of both Σ_0 and Q are selected as 10^{-6}. The diagonal elements of R for all the cases of measurements are defined as 100.

6.2. Selection of sensor frequency

It is well known that a sampling frequency has a great influence on the accuracy of the filter estimates, and its value must be properly chosen depending on system dynamics. For both nonlinear and linear versions of the KF estimator, differentiate equations are approximated using the first-order Euler method; then a sampling period must be chosen considering stability of the numerical approach. For batch distillation, the criteria for the method to prevent the instability is noted by Seader and Henley (1998) as

$$h < \frac{2}{|\lambda|_{\max}} = 2\tau_{\min}$$

It can be seen that an integral interval (h) (or sampling period) is limited to a small step by a fastest response of the process (minimum time constant, τ_{mim}) which is at the end of the operation as can be seen in Fig. 5. In this case, the maximum absolute eigenvalues ($|\lambda|_{\max}$) are about 5400 and 2500 for full- and reduced-state models, respectively. So the sampling time needed for the conventional implementation of the EKF estimator (based on full-state models) is chosen as 2 s. It is noted that the sampling frequency for the novel KF estimator (based on reduced-state models) can be chosen lower than the one needed for the EKF because its $|\lambda|_{\max}$ is lower.

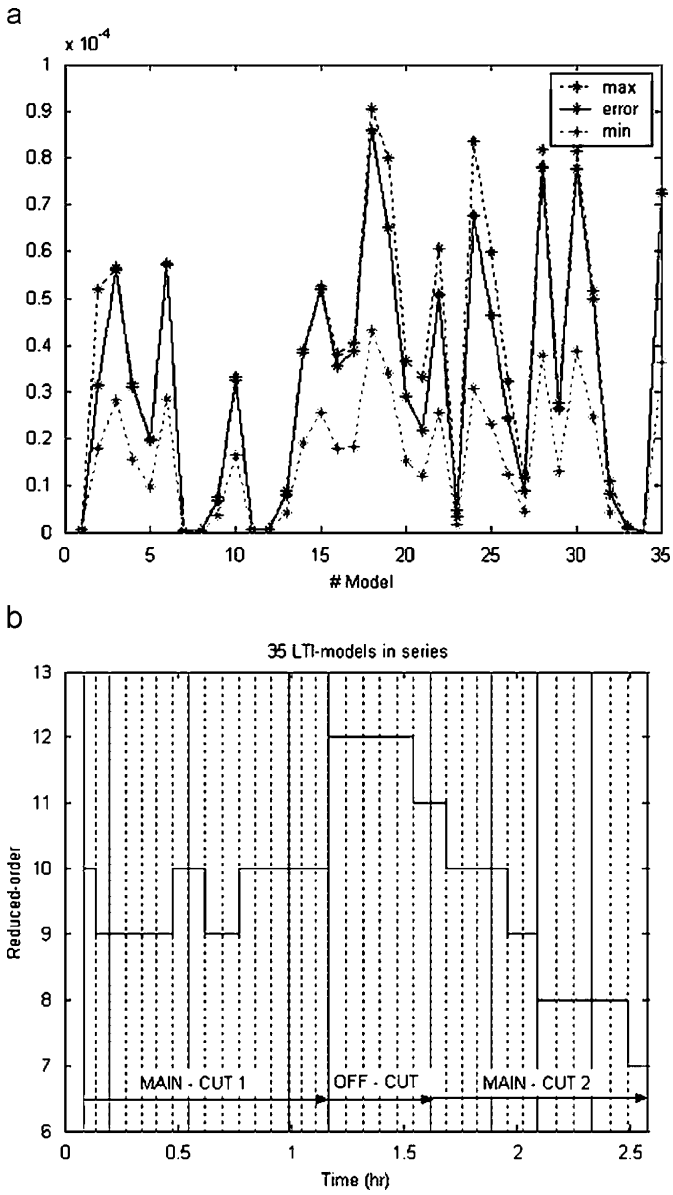


Fig. 4. Reduced models development: (a) error in H_∞ norm and (b) model order.

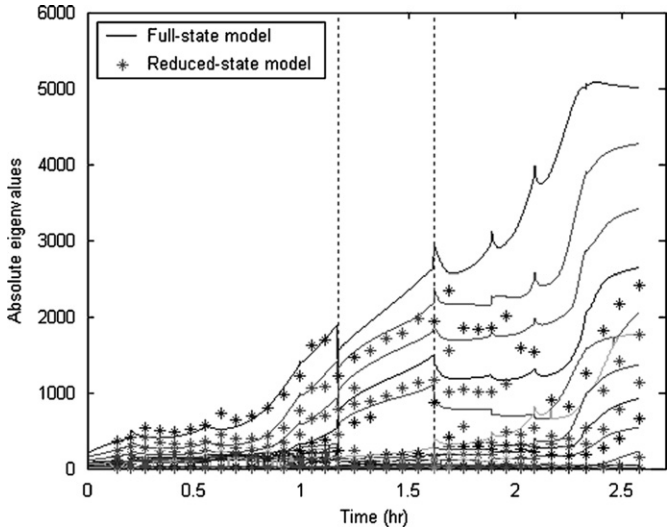


Fig. 5. Absolute eigenvalues of full and reduced models.

Table 5
Parameters which have been varied in the runs

Run	Sampling time	Integrating time h (s)		Initial states	Temperature noise
		Nonlinear	Linear		
1	2	2	2	Exactly	Ideal sensors
2	4	0.4	4	Exactly	Ideal sensors
3	2	2	2	Inexactly	Noise $\pm 1\,K$
4	2	2	2	Inexactly	Noise $\pm 3\,K$

Table 6
Computation effort and IAE values for each run

Run	Computation effort (min)		% Saved	IAE	
	Nonlinear	Linear		Nonlinear	Linear
1	47.588	25.320	46.79	0.101	0.104
2	23.029	14.457	37.22	0.105	0.107
3	47.792	26.670	44.20	0.102	0.161
4	50.315	26.740	46.85	0.103	0.227

Though the sampling time required for the novel estimator is lower than the one needed for the nonlinear estimator, both estimators are tested with sampling time 2 s (Run 1) for evaluating their performances. Table 5 lists the parameters varied in an experimental study and Table 6 gives the computation time as well as integral absolute error (IAE) calculated based on the products. Even though the IAE value in case of the linear estimator is slightly higher the computation time is much lower. It has been found that the computation effort can be saved by over 46% of the one required for the EKF in this case.

Fig. 6 shows the estimation performances of the linear estimator with high sampling time, 4 s (Run 2). The results show that the estimates have reasonable agreement with the actual ones, although lower measurement information is provided. This is because the fast responses at the end of the batch operation are truncated in case of the reduced models as discussed above. However, estimates of the composition obtained by the conventional implement of the EKF estimator with the sampling time of 4 s are poor as seen in Fig. 7 (dotted lines). As the batch changes very rapidly at the end of the operation, the estimator requires more measurement information.

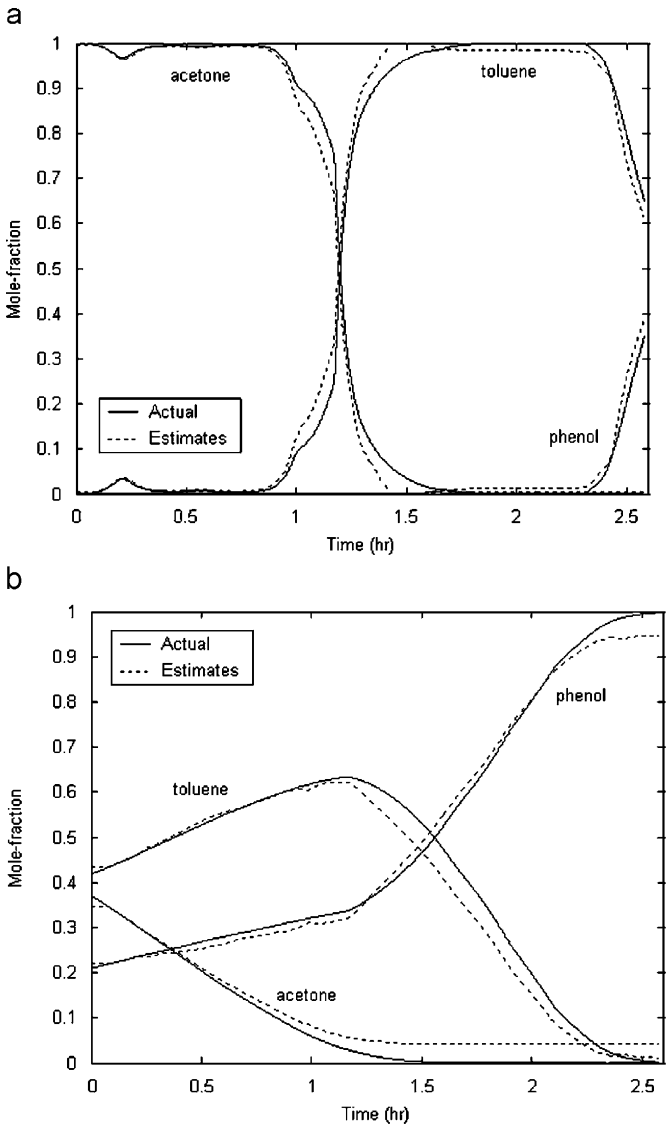


Fig. 6. Estimates of distillate (a) and reboiler (b) compositions using novel KF in Run 2.

6.3. Effect of integrating step for the EKF

As discussed above, the suitable sampling period for the implementation of the estimator is selected considering the stability characteristic of the numerical integrating procedure. If the sensor frequency is high enough, a truncation error of the approximation can be negligible. It has been found that measurement information required for the conventional EKF estimator is remarkably needed for a stiff system such as a batch distillation process. In this subsection, the effect of integrating step size needed for the integrating procedure is tested with the same measurement information. It is expected that with the same sampling, composition estimates during drastic changes of the process can be improved if the integrating step used in the estimator is smaller than the sampling time.

Fig. 7 shows the profiles of the actual composition and the composition estimated by the EKF in a nominal case, varying the integrating step size used for the Euler approximation. The temperature data of every 4 s are used as the input to the EKF algorithm. It can be seen that both the nonlinear estimators give good estimates of acetone. However, in case of the conventional implementation of

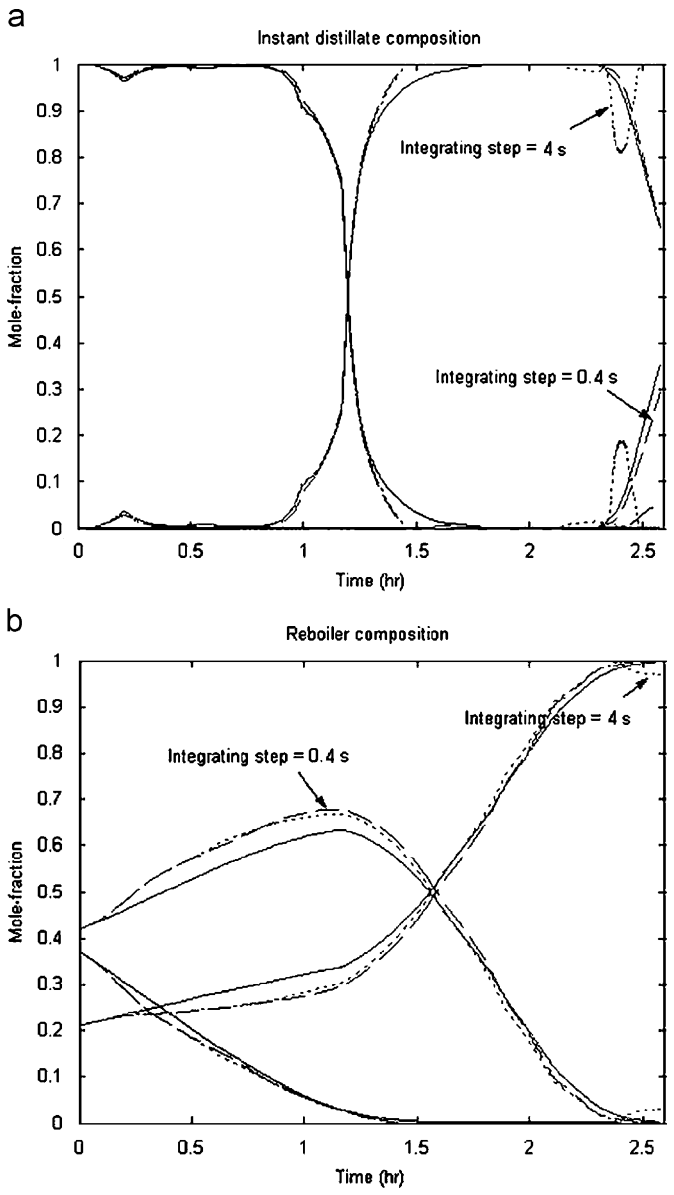


Fig. 7. Distillate (a) and reboiler (b) estimates using EKF (sampling time 4 s).

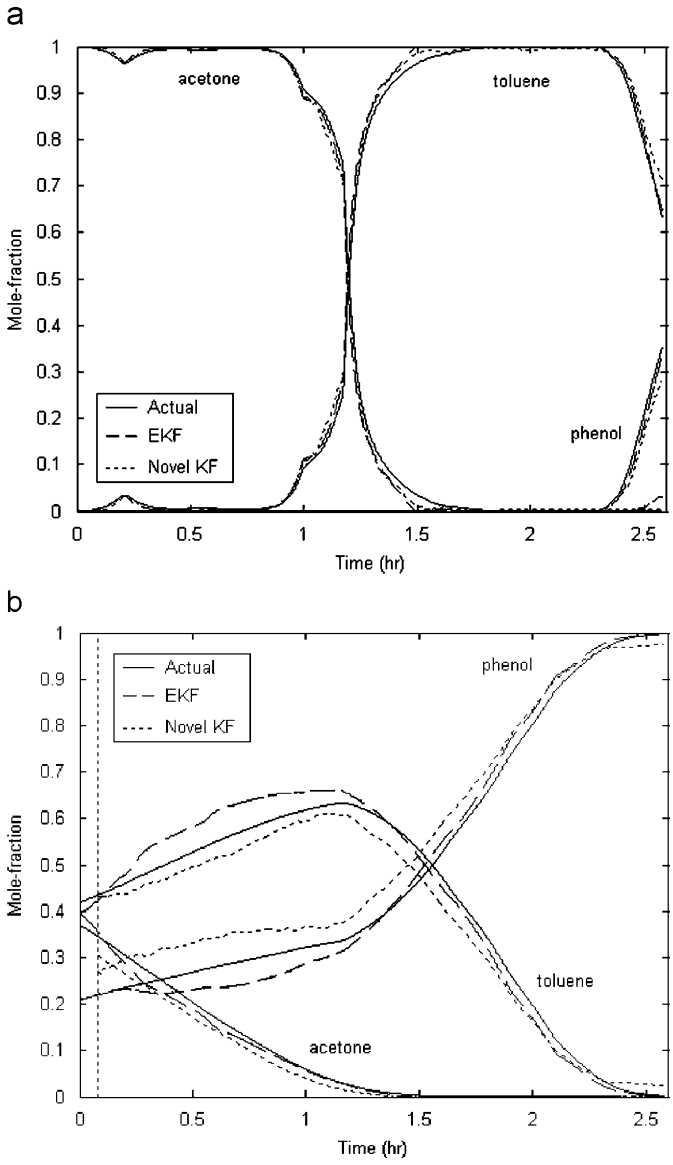


Fig. 8. Composition estimation profiles of distillate (a) and reboiler (b) in Run 3.

the EKF (integrating step 4 s) the estimates of toluene are poor at the end of the operation. The estimation performance is degraded because the integrating method used in the estimator is unstable for the second production. The composition estimates are significantly improved by decreasing the integration interval used in the Euler approach to 0.4 s. The results show that with the constant reflux, the measurement changes rarely effect the product changes.

6.4. Effect of state initialization and noise

For Runs 1 and 2, it is assumed that all initial states are known exactly and can be computed by multiplying the transform matrix with initial full states. However, the initial compositions are rarely known in reality. Keeping all parameters and conditions of Run 1, the robustness of both estimators is tested with respect to the guess values of the initial states. For the EKF estimator, exact initial values of the compositions at all stages are $x_1 = [0.3709, 0.8258, 0.9681, 0.9949, 0.9992, 0.9999, 1]$ and $x_2 = [0.4191, 0.1695, 0.0319, 0.0051, 0.0008, 0.0001, 0]$. Nevertheless, the initial guess values are [0.4, 0.8, 0.9, 1, 1, 1, 1] and [0.4, 0.2, 0.1, 0, 0, 0, 0] for the first and second components, respectively. For the linear estimator, the reduced states are in the incremental changes; then they are initialized by zero for both the productions. In addition, the initial guess of the distillate and reboiler compositions are chosen as [1, 0] and [0.3, 0.43], respectively.

Furthermore, available measurements usually involve statistical error, therefore six sensors are corrupted by a Gaussian white noise with a zero mean and a certain standard deviation. As shown in Fig. 8, both nonlinear and linear estimators still give reasonable estimates of all products with the noise of the standard deviation of 1 K (Run 3). The novel estimator requires the computation effort of only 56% of the one needed for the nonlinear estimator. It has been found that the performances of both linear KF and EKF become worse if the variance of the temperature noise is higher. However, the linear KF is much more sensitive to the higher variance than the EKF. Fig. 9 shows the estimates of both linear KF and EKF with respect to the measurement noise of the standard deviation of 3 K.

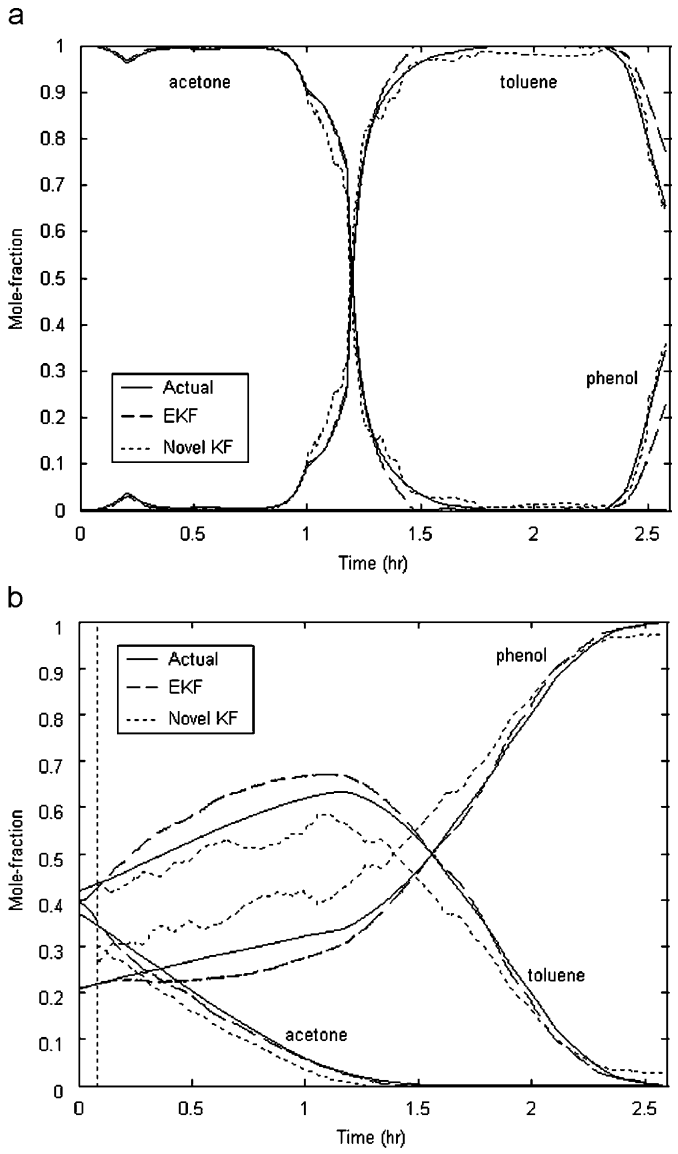


Fig. 9. Composition estimation profiles of distillate (a) and reboiler (b) in Run 4.

7. Conclusion

In this work, both discrete nonlinear and linear versions of a Kalman estimator are developed for inferential composition estimation of a ternary batch distillation. For an EKF estimator, simplified dynamic equations coupled with a bubble-point calculation are employed for an estimator design. Vapor flow rate and holdups of tray and drum are constant for a whole batch operation, in which the values of the parameters are pre-determined in an optimal manner. For a novel linear KF, a set of reduced-order models is developed individually and employed sequentially to predict the whole batch behavior. Pre-scheduling of the models as well as corresponding covariance matrices of a process noise is made. Four important issues are studied: sensor frequency selection, effects of an integrating step size, a state initialization and a measurement noise.

Stability of an Euler approach appears to be an important issue for a sampling period selection of an estimator design. The product estimates at the end of the operation (fast responses) can be improved by decreasing sampling time. It has been found that sampling frequency needed for the estimator based on the reduced model is smaller than the one required for the estimator based on the full model. From the results, the estimation performances of the EKF with the low sampling frequency can be improved by decreasing the integrating step size in the prediction step.

Both estimators give comparative estimation performances even in case of initial guessed conditions and measurement noise. However, the state estimates obtained by the EKF will only converge to the actual values if an accurate thermodynamics model is available. Although the novel estimator performs rather sensitively to the effect of high measurement noise, computation time can be saved by over 44% of the ones required for the EKF estimator. Moreover, the knowledge of the thermodynamic is not required and the augmented states can be initialized easily by using zero values.

Notation

B_0	initial charge in reboiler, kmol
h_j^l	liquid enthalpy of tray j, J/kmol
h_j^v	vapor enthalpy of tray j, J/kmol
H_a	molar holdup of accumulator, kmol
H_j	molar holdup of tray j, kmol (where 1 = reboiler and N = reflux drum)
K_j	a transform matrix of model j as shown in Eq. (20)
L	liquid load, kmol/h
nr	a number of reduced states
nx	a number of stable states
ny	a number of outputs
N	total number of trays including reboiler and condenser
Q	a covariance matrix of process noise
Q_C	heat removed amount in condenser, J/h
Q_R	heat supplied in reboiler, J/h
r	internal reflux ratio
R	a covariance matrix of measurement noise
V	vapor load, kmol/h
x_{ij}	liquid composition of i component in tray j, mole fraction
x_r	a reduced-state vector
y_{ij}	vapor composition of i component in tray j, mole fraction
y_T	a vector of measurable outputs
y_x	a vector of unmeasurable outputs as shown in Eq. (25)

Greek letters

Θ	a state-space realizaion
Σ_0	initial values of a state covariance matrix

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