State Estimation for Batch Distillation Operations with A Novel Extended Kalman Filter Approach

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Abstract—The composition and parameter estimation for batch distillation operations is addressed using a novel extended Kalman filter with unknown inputs without direct feedthrough (EKF-UI-WDF) approach. The major advantage of this approach lies in its capability of estimating states and unknown inputs (e.g. arbitrary deterministic disturbances) simultaneously, whereas the traditional nonlinear filter approaches cannot deal with this problem. As a result, this EKF-UI-WDF approach is able to provide on-line estimation of column compositions, flow rates and other parameters such as the tray efficiency in presence of unknown disturbances and noises. The restrictions of the EKF-UI-WDF are also remarked. Simulation results demonstrate the efficiency of this novel EKF approach comparing with other traditional nonlinear filters and indicate its potential of applications to other complex systems.

I. INTRODUCTION

Batch distillation plays an essential role in chemical plants due to its capability of separating multi-component mixtures and producing high purity components. During the batch operation, the component compositions should be estimated or measured for the control purpose. However, the process model of the batch distillation operation is complex and highly nonlinear. The measurement usually has noises and thus it is difficult to directly measure the compositions. In this regard, nonlinear filtering approaches [1]-[8] are more appropriate to solve this problem.

The best known nonlinear filtering algorithm is the traditional extended Kalman filter (EKF) [1] which is based on linearizing the nonlinear model and measurement equations with the first order Taylor series expansion. Due to its simple implementation and less computation loads, the traditional EKF approach has been applied to batch distillation columns for estimating the compositions (states) on-line with temperature measurements in presence of noises [2]-[5].

However, the EKF algorithm can only approximate the nonlinearities with linear expansions [7]. As an alternative, the unscented Kalman filter (UKF) [6] approximates the nonlinearities at least to the second order with the unscented transformation (UT) method [6]-[7], thus it can provide a more accurate estimation [7]. Both EKF and UKF approaches assume that the noises are with Gaussian distributions and do not apply to general non-Gaussian cases. Some other nonlinear filtering approaches (e.g. particle filter (PF) approach and its improved versions [8]-[9], minimum entropy filter [10], etc.), however, do not require the Gaussian noise assumption. As a result, they can be used for general non-Gaussian cases.

Unfortunately, above nonlinear filter approaches require that both the deterministic inputs in the model and the measurement equations should be known, which sometimes may not be the case in reality (for instance, the time-varying unknown parameters or unmeasured disturbances in the batch distillation operations could both be considered as unknown inputs). The presence of these unknown arbitrary inputs could severely restrict the performances of the classical nonlinear filters since high bias will be introduced into the state estimation due to the uncertainties from the unknown inputs.

On the other hand, it is not always an appropriate idea to treat unknown inputs as random noises to fit those traditional nonlinear filter approaches because (i) the unknown inputs could be signals with an arbitrary type and magnitude, thus it is not suitable to assume them as stable and zero-mean random noises; and (ii) some unknown inputs are required to be estimated for the process control and optimization purposes. In this regard, a joint estimation of the states and unknown inputs for nonlinear stochastic systems becomes a meaningful task, e.g., for batch distillation operations and other industrial processes.

Indeed, the discussion on a joint estimation of states and unknown inputs for linear stochastic systems has been taken for several decades and the most popular way is to solve a constrained optimization problem [11]-[14] where the state unbiasedness is the constraint and a global optimization

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for states and unknown inputs cannot be guaranteed [13]. To avoid the shortcomings of those approaches, an extended Kalman filter with unknown inputs without direct feedthrough (EKF-UI-WDF) approach [15] was proposed for nonlinear stochastic discrete-time systems without direct feedthrough from the unknown inputs to the outputs. The major novelty of the proposed EKF-UI-WDF approach is that the unknown inputs are regarded as a part of the states instead of disturbances (see [11]-[14]). As a result, the EKF-UI-WDF approach can be directly derived from the unconstrained objective function of the traditional EKF (the weighted least squares objective function) and thus becomes a more general version of EKF. Since no prior information of unknown inputs is required, the proposed EKF-UI-WDF is quite suitable for the composition and parameter estimation of batch distillation operations in presence of unknown inputs.

The contributions of this paper can be summarized as follows:

(i) The proposed EKF-UI-WDF approach [15] is applied to batch distillation operations for estimating the states and unknown inputs simultaneously. To the best knowledge of the authors, no previous studies have been made for this application. For comparison, the estimation results of the classical unscented Kalman filter (UKF) and particle filter (PF) are also presented.

(ii) This paper discusses the identification of model parameters (such as the tray efficiency), which is important in batch distillation operations but has not been investigated in the previous research [2]-[5].

(iii) To efficiently reduce the computation load and improve the estimation performance, an new procedure (see Eq.(34) for details) are provided to separately estimate the important states (compositions and parameters) and other profiles (such as liquid and vapor flow rates, temperatures, etc.) by the combination of the EKF-UI-WDF approach and a similaric (solver) for batch distillation.

The paper is organized as follows: Section II describes the process model of batch distillation columns. Section III presents the state equations for the purpose of composition estimation. Section IV revisits the EKF-UI-WDF approach. Section V presents the simulation results to demonstrate the effectiveness of the EKF-UI-WDF approach. Section VI concludes the paper and gives suggestions in the future work.

II. PROCESS MODEL OF BATCH DISTILLATION COLUMNS

The general nonlinear process model for batch distillation operations involves dynamic component and energy balances as well as algebraic equations representing the vapor–liquid equilibrium and physical properties. The main assumptions adopted for the process model development are given as follows:

1. Liquid on the tray is perfectly mixed and incompressible.
2. The molar vapor hold-up is negligible compared with the molar liquid hold-up.
3. The liquid and vapor leaving each plate are in the thermal equilibrium (same temperature) but not in phase equilibrium (the Murphree tray efficiency < 100%).
4. The stages are numbered from the top to the bottom of the column.

The equations describing the process are given as follows:

Reflux Drum (Subscript 1):

\[
\begin{align*}
\frac{d \mathrm{HU}_i}{dt} &= V_2 - D - L_1 + \mathrm{HU}_i \Delta R_i \\
\frac{d \left( \mathrm{HU}_i x_{1,i,j} \right)}{dt} &= V_2 y_{2,i,j} - (D + L_1)x_{1,i,j} + \mathrm{HU}_i R_{1,i,j} , \quad j = 1, \ldots, N_c \\
\frac{d \left( \mathrm{HU}_i L_{U,i,j} \right)}{dt} &= V_2 \sum_{j=1}^{N_c} \left[ H_{V2,i,j} - (D + L_1) \sum_{j=1}^{N_c} \left[ H_{U,i,j} x_{1,i,j} \right] + Q_i \right]
\end{align*}
\]

Trays (Subscript \( i, i = 2, 3, \ldots, N_1 - 1 \)):

\[
\begin{align*}
\frac{d \mathrm{HU}_i}{dt} &= V_{i+1} + L_{i-1} - V_i - L_i + \mathrm{HU}_i \Delta R_i \\
\frac{d \left( \mathrm{HU}_i x_{i,i,j} \right)}{dt} &= V_{i+1} y_{i+1,i,j} + L_{i-1} x_{i-1,i,j} - V_i y_{i,i,j} - L_i x_{i,i,j} + \mathrm{HU}_i R_{i,i,j} , \quad j = 1, \ldots, N_c \\
\frac{d \left( \mathrm{HU}_i L_{U,i,j} \right)}{dt} &= V_{i+1} \sum_{j=1}^{N_c} \left[ H_{V,i+1,j} y_{i+1,j} \right] + L_{i-1} \sum_{j=1}^{N_c} \left[ H_{U,i,j} x_{i,j} \right] - V_i \sum_{j=1}^{N_c} \left[ H_{V,i,j} y_{i,j} \right] - L_i \sum_{j=1}^{N_c} \left[ H_{U,i,j} x_{i,j} \right] + Q_i
\end{align*}
\]

Reboiler (Subscript \( N_1 \)):

\[
\begin{align*}
\frac{d \mathrm{HU}_{N_1}}{dt} &= L_{N_1-1} - V_{N_1} - L_{N_1} + \mathrm{HU}_{N_1} \Delta R_{N_1} \\
\frac{d \left( \mathrm{HU}_{N_1} x_{N_1,j} \right)}{dt} &= L_{N_1-1} x_{N_1-1,j} - V_{N_1} y_{N_1,j} - L_{N_1} x_{N_1,j} + \mathrm{HU}_{N_1} R_{N_1,j} , \quad j = 1, \ldots, N_c \\
\frac{d \left( \mathrm{HU}_{N_1} L_{U,1,j} \right)}{dt} &= L_{N_1-1} \sum_{i=1}^{N_1} \left[ H_{L,i,j} x_{N_1,j} \right] - V_{N_1} \sum_{i=1}^{N_1} \left[ H_{V,i,j} y_{N_1,j} \right] - L_{N_1} \sum_{i=1}^{N_1} \left[ H_{U,i,j} x_{N_1,j} \right] + Q_{N_1}
\end{align*}
\]

in which \( x_{i,j} \) and \( y_{i,j} \) (\( i = 1, \ldots, N_1, j = 1, \ldots, N_c \)) are the liquid and vapor mole fractions for jth composition in the reflux drum, all trays and reboiler, from the top to the bottom of the column, respectively; \( \mathrm{HU}_i \) (\( i = 1, \ldots, N_1 \)) are the
hold-ups of all stages, respectively; \( H_{Li,j} \) and \( H_{Vi,j} \) (i = 1, \( \cdots \), \( N_t \), j = 1, \( \cdots \), \( N_c \)) are the liquid and vapor enthalpy for jth composition in all stages; D and \( L_i \) are the liquid flow withdrawal and reflux flow rate from the reflux drum, respectively; \( L_i \) and \( V_i \) (i = 2, \( \cdots \), \( N_t \)) are the liquid and vapor flow rates from all trays and reboiler, respectively; \( \Delta R_i \) (i = 1, \( \cdots \), \( N_t \)) are the reactive incremental rate for all the stages; \( R_{i,j} \) are the reactive incremental rate for jth composition in all stages; and \( Q_i \) (i = 1, \( \cdots \), \( N_t \)) are the reactive or external heat rate (power).

The vapor-liquid relationship is considered as follows

\[
y_{i,j} = \eta_i K_{i,j} x_{i,j} + (1-\eta_i) y_{i+1,j} ; \quad K_{i,j} = \frac{p_{i,j}^0 y_{i,j}}{p_i} \quad (10)
\]

where \( \eta_i \) is the tray efficiency for ith (i = 2, \( \cdots \), \( N_t \) - 1) tray and reboiler (i = \( N_t \)), \( P_i \) and \( T_i \) are the plate pressure and temperature at ith (i = 1, \( \cdots \), \( N_t \) ) plate; \( p_{i,j}^0 \) and \( \gamma_{i,j} \) are the component vapor pressure and activity coefficient (computed with Uniquac model) at ith (i = 1, \( \cdots \), \( N_t \) ) plate for jth (j = 1, \( \cdots \), \( N_c \)) component, respectively. The relationship between \( p_{i,j}^0 \) and \( T_i \) can be described by the Antoine equation:

\[
p_{i,j}^0 = \frac{10^{A_j-B_j/(T_i-273.15)+C_j}}{750.06}
\]

where \( A_j \), \( B_j \) and \( C_j \) are the Antoine constants for jth composition. In summary, the model is composed of a nonlinear differential-algebraic equation (DAE) system with a high dimension.

III. STATE EQUATIONS FOR COMPOSITION ESTIMATION

To relieve the computation load and improve the estimation precision for the application of the EKF-UI-WDF approach, it is desirable to reduce the dimension of the nonlinear state equations from the general process model presented in Section II. Consequently, it is not wise to include all of the unknown batch distillation profiles in the state vector. For instance, the component compositions at each stage and some important parameters such as the tray efficiency should be considered. The other profiles, including flow rates and temperatures along the column, can be indirectly obtained from the estimated states by the dynamic equations given in Section II.

Based on this idea the general process model of batch distillation operations can be condensed to a nonlinear dynamic model with a lower dimension. Consider that the component compositions are constrained by the relationship

\[
\sum_{i=1}^{N_t} x_{i,j} = 1 \quad (i = 1, 2, \cdots, N_t), \quad n \quad (Nc-1)*N_t + N_p \)

A state vector is given as follows:

\[
Z(t) = [x_{1,1}, \cdots, x_{N_t,N_c-1}, x_{2,1}, \cdots, x_{N_t,N_c-1}, \cdots, x_{N_t,N_c}, x_{N_t,N_c-1}, \cdots, x_{N_t,N_c-1}, x_{N_t,N_c}, \theta_1, \cdots, \theta_{N_t}]^T
\]

where \( \theta_i \) (i = 1, 2, \( \cdots \), \( N_p \)) are the parameters to be estimated. The state model equations are then obtained by substituting the vapor-liquid relationship in Eq.(10) into Eqs.(2), (5) and (8) (the variations of all hold-ups are assumed known), as follows

\[
Z(t) = g_c(Z(t), X(t), u(t), u^*(t)) + w(t) \quad (13)
\]

where \( g_c \) denotes a nonlinear continuous function; \( X(t) \) the m-vector which contains the column profiles to be indirectly estimated.

Since the measurements are usually the temperatures of some stages \([2]-[5]\), the measurement equations can be obtained from Eq.(11), i.e.

\[
y_k = h_k^0 + v_k \quad (14)
\]

where the elements of \( h_k = h(Z_k, X_k, u_k, k) \), \( h_{jk} \) are the temperatures \( T_{jk} \) of jth stages (1 \( \leq j \leq N_t \)) at t = k\( \Delta t \) (\( \Delta t \) is the sampling instant), as follows

\[
h_{jk} = T_{jk} = \frac{B_j}{A_j \log_{10}(750.06p_{i,j}^0)} + 273.15 - C_j \quad (15)
\]

Substituting the approximation \( \frac{dZ}{dt}|_{t=k\Delta t} = \frac{Z_k - Z_{k-1}}{\Delta t} \) into Eq.(13), the following nonlinear discrete state equations can be obtained,

\[
Z_k = g_{k-1} + w_{k-1} \quad (16)
\]

where

\[
g_{k-1} = g(Z_{k-1}, X_{k-1}, u_{k-1}, u^*_{k-1}, k-1) \quad (17)
\]

where \( Z_k \) and \( Z_{k-1} \) are n-state vectors at t = k\( \Delta t \) and t = (k - 1)\( \Delta t \), \( X_k \) and \( X_{k-1} \) are m-vectors at t = k\( \Delta t \) and t = (k - 1)\( \Delta t \), respectively; \( v_k \) is p-observation (measured) output vector at t = k\( \Delta t \); \( u^*_{k-1} \) is r-unknown input vector at t = (k - 1)\( \Delta t \); \( u_k \) and \( u_{k-1} \) are s-known control input vectors at t = k\( \Delta t \) and t = (k - 1)\( \Delta t \), respectively; \( w_{k-1} \) and \( v_k \) are n-model noise (uncertainty) and p-measurement noise vectors assumed to be mutually independent Gaussian white sequences with zero means and autocovariance functions \( E[w_{k-1}w_{k-1}^T] = Q_{k-1} \) and \( E[v_k v_k^T] = R_k \), respectively.

In the following the bold face letter represents either a vector or a matrix.
IV. THE REVISIT OF EKF-UI-WDF APPROACH

The EKF-UI-WDF approach [15] can be used to estimate of unknown state and input vectors $Z_{k}$ and $u_{k-1}$ at $t = k \Delta t$ given the observations $(y_{1}, y_{2}, \ldots, y_{k})$, denoted as $\hat{Z}_{k|k}$ and $\hat{u}_{k-1|k}$, respectively. The derivation of EKF-UI-WDF is briefly explained in the following.

First, the nonlinear functions $g_{k-1}$ in Eq.(17) and $h_{k}$ in Eq.(14) is linearized to give,

$$g_{k|-1} = g(\hat{Z}_{k|-1}, \hat{X}_{k}, u_{k-1}, k^{-1}) + B_{k-1} h_{k|-1}(u_{k-1} - \hat{u}_{k-2|k-1}) \tag{18}$$

$$h_{k} \approx \hat{h}_{k|k-1} + H_{k|k-1}(Z_{k} - \hat{Z}_{k|k-1}) \tag{19}$$

where

$$\hat{g}_{k-1|k-1} = g(\hat{Z}_{k-1|k-1}, \hat{X}_{k-1|k-1}, \hat{u}_{k-1|k-1}, k^{-1}) \tag{20}$$

$$\hat{h}_{k|k-1} = h(\hat{Z}_{k|k-1}, \hat{X}_{k|k-1}, u_{k-1}, k) \tag{21}$$

Next, the estimates $\hat{Z}_{k|k}$ and $\hat{u}_{k-1|k}$ can be determined by minimizing the objective function of the summed square error between $y_{i}$ and $h_{i}$ $(i = 1, 2, \ldots, k)$, i.e.,

$$J_{k} = \sum_{i=1}^{k} (y_{i} - h_{i})^{2} \tag{22}$$

where $W_{k}$ is a $(pk \times pk)$ weighting matrix which is defined as the inverse of the covariance model for model and measurement noises; $\Lambda_{i} = y_{i} - h_{i}$ is a p-output error vector at $t = i \Delta t$ $(i = 1, 2, \ldots, k)$ and $\Lambda_{k} = [\Lambda_{1}^{T}, \Lambda_{2}^{T}, \ldots, \Lambda_{k}^{T}]^{T}$ is a pk-vector. Minimized $J$ with respect to the unknown extended state vector $Z_{e,k}$ with respect to the unknown extended state vector $Z_{e,k}$ at $t = k \Delta t$ as follows

(i.e. $\hat{Z}_{e,k|k}$ satisfies $\frac{\partial J_{k}}{\partial Z_{e,k}} |_{Z_{e,k}=\hat{Z}_{e,k|k}} = 0)$:

$$\hat{Z}_{e,k|k} = P_{e,k} [A_{e,k}^{T} W_{k} V_{k}]^{-1} P_{e,k} = [A_{e,k}^{T} W_{e,k} A_{e,k}]^{-1} \tag{23}$$

where $\hat{Z}_{e,k|k} = [\hat{Z}_{k|k}^{T} \hat{u}_{1|k}^{T} \hat{u}_{2|k}^{T} \cdots \hat{u}_{k-1|k}^{T}]^{T}$, $Y_{k}$ is a pk-known vector and $A_{e,k}$ is a [pk x (n+(k-1)r)] known matrix.

After a tedious derivation procedure, the desirable recursive solutions for $\hat{Z}_{k|k}$ and $\hat{u}_{k-1|k}$ can be obtained by following steps:

Step I: Prediction

$$\hat{Z}_{k|k-1} = \hat{g}(\hat{Z}_{k-1|k-1}, \hat{X}_{k-1|k-2}, u_{k-1|k-1}, k-1) \tag{27}$$

where $\hat{Z}_{k|k-1}$ and $\hat{u}_{k-1|k-1}$ are the estimations of states and unknown inputs at $t = (k-1) \Delta t$.

Step II: Gain Computation

The computations of the gain matrices for the estimations of states and unknown inputs at $t = k \Delta t$ are respectively given by

$$K_{Z,k} = P_{Z,k|k-1} H_{k|k-1}^{T} [R_{k} + H_{k|k-1} P_{Z,k|k-1} H_{k|k-1}^{T}]^{-1} \tag{28}$$

$$S_{k} = [B_{k-1}^{T} P_{Z,k-1} H_{k|k-1} R_{k-1}^{-1}(I_{p} - H_{k|k-1} K_{Z,k})]^{T} \tag{29}$$

$$H_{k|k-1} P_{Z,k-1}^{T} \tag{30}$$

where $P_{Z,k|k-1} = G_{k-1|k-1} P_{Z,k-1|k-1} G_{k-1|k-1}^{T} + Q_{k-1}$ is the autocovariance function of the model noise process vector $w_{k-1}$.

Step III: Update

In this step, the estimations of state and unknown inputs at $t = k \Delta t$, $\hat{Z}_{k|k}$ and $\hat{u}_{k-1|k}$ are updated from the combination of the state prediction and current measurement:

$$\hat{Z}_{k|k} = \hat{Z}_{k|k-1} + K_{Z,k} [y_{k} - h(\hat{Z}_{k|k-1}, \hat{X}_{k|k-1}, u_{k}, k)] \tag{31}$$

$$\hat{u}_{k-1|k} = S_{k} B_{k-1}^{T} P_{Z,k-1|k-1} G_{k-1|k-1} - (I_{p} - H_{k|k-1} K_{Z,k}) \tag{32}$$

The covariance matrix $P_{Z,k|k-1}$ in Eq.(30) is updated at $t = (k-1) \Delta t$:

$$P_{Z,k-1|k-2} = (I_{n} - K_{Z,k-1} H_{k|k-2}) P_{Z,k-1|k-2} + B_{k-2}^{*} S_{k} B_{k-2}^{*} + (I_{n} - K_{Z,k-1} H_{k|k-2})^{T} \tag{33}$$

where $K_{Z,k-1}$, $S_{k-1}$ and $P_{Z,k-1|k-2}$ are obtained from Eqs.(28)-(30) by replacing k by k-1, respectively.

Remark 1: It can be seen from Eqs.(30) that the estimation of $X_{k}$, $\hat{X}_{k|k-1}$ is required for the state estimation in addition
to \( \hat{Z}_{k|k-1} \). To obtain \( \hat{X}_{k|k-1} \) and \( \hat{Z}_{k|k-1} \) simultaneously, instead of using Eq.(27), the following step is executed, i.e.,

\[
g(Z(t), \hat{Z}(t), X(t), \hat{X}(t)) = 0; \quad t_{k-1} \leq t \leq t_k
\]

Initial values: \( \hat{Z}_{k-1|k-1} \) and \( \hat{X}_{k-1|k-2} \) at \( t = t_{k-1} \)

\[
\Rightarrow \hat{Z}_{k|k-1} \quad \text{and} \quad \hat{X}_{k|k-1} \quad (34)
\]

where \( g(Z(t), \hat{Z}(t), X(t), \hat{X}(t)) = 0 \) represents the process model given in Section II. This step can be realized by using a simulator for the batch distillation operation.

Remark 2: By checking the existence condition for

\[
P_{e,k} = [A_{e,k}^T W_{e,k} A_{e,k}]^{-1} \quad (\text{see Eq.(26)}),
\]

it can be concluded that the major restriction of EKF-UI-WDF is that the number of measurements (\( p \)) should be larger than the number of unknown inputs (\( r \)).

V. SIMULATION RESULTS

In this section, a semi-batch distillation operation for the separation of a binary Tuluol/Cyclohexan mixture is used to verify the EKF-UI-WDF approach. The specifications for the distillation operation are listed in Table I. To imitate the unknown input during the distillation operation, an extra Tuluol/Cyclohexan mixture is fed into the semi-batch distillation column at the 10th stage (the inlet) from \( t = 10 \) sec. to \( t = 30 \) sec. The simulation of the distillation operation lasts 30 seconds for the state estimation purpose (though the real distillation operation usually costs several hours).

To implement the composition estimation with the EKF-UI-WDF approach, the \( i \)th composition (\( x_{i,1} \)) of Cyclohexan and the tray efficiency for all stages (\( \eta \)) are denoted as \( z_{i} \) (\( i = 1, 2, \ldots, 20 \)) and \( z_{21} \), respectively. Let \( \Delta t = 1 \) sec., the discrete condensed state equations given in Eq.(16) are obtained where the process noises are the Gaussian noises (zero mean and standard deviation 0.005) and the measurements are assumed to be the temperature at 1st, 10th and 20th stages which are corrupted with random Gaussian noises (zero mean and standard deviation 0.1°C).

The theoretical value of the unknown input \( u_{k-1}^* \) in Eq.(17) is set 0 at \( t = 0 - 10 \) sec. Based on Eq.(5), at \( t = 10 - 30 \) sec., the theoretical \( u_{k-1}^* = \Delta t^* F_{10,1} / H_{10} = 0.1 \) where \( F \) is the flow rate of the extra mixture fed into the 10th stage (the inlet), \( x_{10,1} \) is the Cyclohexan composition of the extra mixture and \( H_{10} \) is the hold-up of the 10th stage.

Unknown quantities to be estimated by the EKF-UI-WDF approach are: (i) the 21-state vector \( z_{k} \); and (ii) the unknown input \( u_{k-1}^* \). The initial states for the estimation are assumed to have 5% deviation from the real values and the initial covariance matrix are defined as \( P_{00} = (21 \times 21) \) diagonal matrix = \( \text{diag} \{10^{-4}, \ldots, 10^{-4}, 1\} \), the autocovariance matrices for model and measurement noises as \( Q_{k-1} = 10^{-5} I_{21} \) and \( R_{k} = 0.1 I_{3} \), respectively. After the state update at each step (see Eq.(31)), the other column profiles such as vapor and liquid flow rates as well as the temperature at each stage, \( V_i, L_i \) and \( T_i \) (\( i = 1, 2, \ldots, 20 \)) can be calculated (indirectly estimated) by Eq.(34).

Based on EKF-UI-WDF given by Eqs.(27)-(34), the states and unknown inputs are estimated simultaneously. For comparison, the unscented Kalman filter (UKF) [7] and particle filter (PF) [8] (particle number = 200) are also used for the batch distillation operation problem. Due to the limit
of space, only the estimation results of $Z_{10}$ (the Cyclohexan composition at the inlet stage) and $Z_{21}$ (the tray efficiency $\eta$) are presented in Fig. 1. The estimated unknown input with EKF-UI-WDF approach is also presented in Fig. 2. Meanwhile, to compare the consistency of the three filters, their normalized mean-squared estimation error (MSEE) (i.e. the actual MSEE (calculated from 100 Monte Carlo simulations) is divided by the estimated MSEE (the diagonal element of the state covariance matrix)) for $Z_{10}$ is presented in Fig. 3 (the figure of the normalized MSEE for $Z_{21}$ is similar to Fig. 3 thus it is omitted here).

It can be observed from Figs. 1-3 that (i) EKF-UI-WDF can track the states $Z_k$ (including the tray efficiency parameter $\eta$) and unknown input $u_{k-1}^*$ well; (ii) the UKF and PF have better performances (lower state estimation errors (see Fig. 1), and higher consistencies where their normalized MSEEs are closer to 1 (see Fig. 3) than the one of EKF-UI-WDF when $u_{k-1}^* = 0$ (at $= 0 – 10$ sec.); and (iii) the UKF and PF have worse performances than the one of EKF-UI-WDF when $u_{k-1}^* \neq 0$ (at $= 10 – 30$ sec.). Consequently, it can be concluded that (i) the traditional UKF and PF prevail the EKF approach when all inputs are known (which has already been proved by numerous previous work, e.g. [7]); and (ii) the proposed EKF-UI-WDF performs better than the traditional UKF and PF in presence of the unknown input (this is also reasonable because the negative effect of the unknown input counteracts the advantages of the traditional UKF and PF over the EKF-UI-WDF). Finally, the simulation results indicate that one possible direction for our future work is to combine the advantages of those advanced nonlinear filter approaches and develop more accurate state estimation in presence of unknown inputs.

VI. CONCLUSIONS

In this paper, a novel extended Kalman filter with unknown inputs without direct feedthrough (EKF-UI-WDF) approach is revisited and applied to batch distillation operations for composition and parameter estimation in presence of unknown inputs. Simulation results demonstrate that the EKF-UI-WDF approach perform well in presence of unknown inputs comparing with other traditional nonlinear filter approaches. The next step is to extend EKF-UI-WDF to treat large-scale complex DAE systems.

REFERENCES