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In the control of batch distillation columns, one of the problems is the difficulty in monitoring the compositions. This problem can be handled by estimating the compositions from readily available online temperature measurements using a state estimator. In this study, a state estimator that infers the product composition in a multicomponent batch distillation column (MBDC) from the temperature measurements is designed and tested using a batch column simulation. An extended Kalman filter (EKF) is designed as the state estimator and is implemented for performance investigation on the case column with eight trays separating the mixture of cyclo-hexane, -heptane and toluene. EKF parameters of the diagonal terms of process noise covariance matrix and those of measurement model noise covariance matrix are tuned in the range where the estimator is stable and selected basing on the least IAE score. Although NC-1 temperature measurements is sufficient considering observability criteria, using NC measurements spread through out the column homogeneously improves the performance of EKF estimator. The designed EKF estimator is successfully used in the composition—feedback inferential control of MBDC operated under variable reflux-ratio policy with an acceptable deviation of 0.5–3% from the desired purity level of the products.

'Batch distillation is generally used as a separation unit in the fine speciality chemicals, pharmaceuticals, biochemical and food industries. The demand and the uncertainty in specifications for these chemicals has increased recently, which increased the popularity of the use of batch distillation' (Barolo and Cengio, 2001; Kim and Ju, 1999). Instead of using many continuous columns in series, multiple products can be obtained from a single batch distillation column during a single batch run. Moreover, batch distillation processes can easily handle variations both in the product specifications and in the feed compositions. This flexibility of batch distillation processes provides the ability to cope with a market characterized by short product life times and strict specification requirements.

In batch distillation, the operation of the column with optimized operation scenario; including reflux ratio policy, switching times, and method of recycling, is required to be realized in a convenient control system. However, in order to employ the operation scenario; the designed controller will require continuous information flow from the column, including the compositions throughout the column or temperatures reflecting the composition knowledge. The reason for this requirement is that, the value of reflux ratio and switching between product and slop cut distillations are optimized which are subject to the composition profile along the column and obtained as a function of it. Therefore, the need for knowledge of current composition in the column becomes obvious.

The composition knowledge can be generated by means of direct composition analysers in the control of a batch distillation column. Although there is a great development in the technology of online composition analysers, such as gas chromatography, they bring large measurement delays and high investment and maintenance costs (Mejdell and Skogestad, 1991; Oisiovici and Cruz, 2000; Venkateswarlu and Avantika, 2001). The most popular alternative to the composition controllers utilizing analysers is standard temperature feedback controllers. Although temperature measurements are inexpensive and have negligible measurement delays, they are not accurate indicators of composition (Mejdell and Skogestad, 1991). Another alternative is inferential control systems incorporating state estimators which use secondary temperature measurements.

State estimation can be defined as the process of extracting information from data which contain valuable

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Assumptions made in the model development.

Negligible vapour holdup
Constant volume of tray liquid holdup
Constant liquid molar holdup in the reflux-drum
Total condenser
Negligible fluid dynamic lags
Linear pressure drop profile
Murphree tray efficiency
Approximated enthalpy derivatives
Adiabatic operation

Summary of MBDC rigorous model equations.

Compositions and holdups

$$_{1} = {}^{0} - \sum_{=2}^{+2} - \int$$

derivation and variations in the molal tray holdup will be provided by variations in the liquid density that is a function of composition, temperature and pressure. Instead of using ideal tray assumption, to represent the non-ideality in the phase equilibrium, Murphree tray efficiency formulation is employed assuming the temperature equilibria between the vapour and the liquid phases. Consequently, the basic assumptions made in the simulation model development are summarized in Table 1.

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The EKF is defined as 'optimal recursive data processing algorithm' (Maybeck, 1979), handling the estimation issues in the nonlinear system theory. EKF uses the nonlinear model of the system given by equation (1)

$$\dot{\_}(\ ) = \_(\_(\ ), \_(\ ), \ ) + (\ )\_(\ ) \quad (1)$$

where is the vector of the nonlinear system functions and the noise process, $\_(\ )$ is modelled as white Gaussian noise with statistics

$$\{\_(\ )\} = 0 \quad (2)$$

$$\{\_(\ )\_(\ ')'\} = \begin{cases} (\ ), & = ' \\ 0, & \neq ' \end{cases} \quad (3)$$

and the nonlinear measurement model written as

$$\_(_k) = [\_(_k), _k] + \_(_k) \quad (4)$$

where is the vector of the nonlinear measurement functions and the noise process, $\_(_k)$ is modelled as white Gaussian noise with statistics

$$\{\_(_k)\} = 0 \quad (5)$$

$$\{\_(_k)\_(_l)'\} = \begin{cases} \_(\ ), & _k = _l \\ 0, & _k \neq _l \end{cases} \quad (6)$$

The EKF has a two-step recursive calculation algorithm. The first named as is responsible to calculate the prediction of the state at the current time using the best state estimate at the previous time step. The second is named as and updates the prediction found in the first stage using the measurements taken from the actual process and calculates the best state estimate. The propagation stage integrates the state and error covariance derivatives (see Table 4: Propagation section) from the previous time step t_{k-1} to the current time t_k and uses the best state estimate $\hat{x}^+(t_{k-1})$ and its error covariance $P^+(t_{k-1})$ at the previous time step t_{k-1}, in order to calculate the prediction of the state, $\hat{x}^-(t_k)$ and its error covariance $P^-(t_k)$ at the current time step t_k. The update stage utilizes the equations given in Table 4 (Update section), and updates the prediction of the state $\hat{x}^-(t_k)$ and its error covariance $P^-(t_k)$ at the current timestep t_k.

Lastly, in order to initiate the EKF algorithm, the information of initial conditions is required and stated by $\hat{\underline{\ }}_0$ for the states and by $\underline{\ }_0$ for the error covariances.

As a result, the nonlinear models for the system and for the temperature measurements are to be developed in the form required for EKF algorithm. However, the model developed for rigorous simulation of the batch column is not suitable for realistic situation in order to be implemented in EKF algorithm. For the reason that it is difficult to obtain the required values of vapor and liquid flowrates and tray holdups with time. In addition, the complexity of the simulation model requires high computational time and memory. Therefore, the rigorous column model for simulation is to be simplified and then the obtained nonlinear model is to be linearized to achieve the Jacobian matrix both for the system and the measurement processes.

Some additional assumptions are needed for the simplification of the rigorous simulation model of MBDC. These assumptions are constant molar holdup on trays, disregard of the energy dynamics in the column, ideal trays, and use of Rault's Law with Antoine's vapour pressure correlation for vapour–liquid equilibrium (VLE) description. As a result, the vapour flowrates throughout the column become equal as well as the liquid flowrates. The simplified model equations for MBDC are given in Table 5.

Next, the nonlinear models in EKF given by equations (1) and (4) are defined in terms of states, inputs and outputs of the column-simplified-model by equations (10) to (16) as

$$\dot{\underline{\ }}(\ ) = \underline{\ }(\underline{\ }(\ ), \underline{\ }(\ ), \ ) + \underline{\ }(\ ) \tag{10}$$

where

$$\underline{\ } = [\ _{11} \cdots \ _{1NC}, \ldots, \ _{NT+2,1} \cdots \ _{NT+2,NC}]^{TNT} \tag{11}$$

$$\underline{\ } = [\dot{\ }_{11} \cdots \dot{\ }_{1NC}, \ldots, \dot{\ },$$

are evaluated analytically. Their expanded forms and the details of the derivation are given by Yıldız (2002).

Consequently, all the information required for EKF estimator has been obtained. This information incorporates nonlinear and linearized models for the system of MBDC and the measurement process given respectively by _, _, _′, _′.

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The case column for simulation is the one which was simulated by Mujtaba and Macchietto (1993) in their study on the subject of optimal operation of MBDC. The column is used to separate the mixture of cyclo-hexane, -heptane and toluene. The sketch of the column can be seen in Figure 1 and the design specifications of the column are listed in Table 6.

The batch distillation column is under the perfect control of reflux-drum level and has two degrees-of freedn036(degre)-9(es0TfT*94n)-61nipmulation of 3Tdt8.910rboiler heat load, $_1$ and reflux-ratio,

Figure 3. Mismatch between the modified process model and the EKF model.

As a result it is decided that in the model development, the most important part is the selection of VLE formulation.

The simulation test runs for tuning the EKF is done without considering any changes in VLE relationship of the EKF model because VLE relationship does not change the effects of tuning parameters on the performance of EKF. Further, it is aimed to obtain the optimum values for these parameters in the worst case (i.e., process/model mismatch). The tuning parameters for EKF are the diagonal terms of process noise covariance matrix, q, and the diagonal terms of measurement model noise covariance matrix, r. Also, the effect of number of measurement points, and measurement period, Δt_m will be illustrated. It is known that, in initialization of the EKF, initial estimates vector, $\underline{x}_0$ and its error covariance vector, $\underline{P}_0$ are also important. These will be discussed also.

In all of the simulation test runs, the integral absolute error (IAE) is chosen as the performance criteria reflecting the fitness of the EKF design parameters. The formulation of IAE between the actual and the estimated fractions of a component is given in equation (21)

$$IAE_i = \int_0^{t_f} |\hat{x}_i(t) - x_i(t)|\,dt \tag{21}$$

where $\hat{x}_i(t)$ is the estimated composition of ith component, $x_i(t)$, the actual one and t_f, the total time of batch. In the performance evaluation, instead of analysing the IAE scores of each component separately, the sum of the IAE scores of the components is selected. Moreover, this total score is calculated both for the reflux-drum and the reboiler composition estimations as given by equations (22) and (23)

$$IAE_{RD} = \sum_{i=1}^{N} IAE_i \tag{22}$$

$$IAE_{RB} = \sum_{i=1}^{N} IAE_i \tag{23}$$

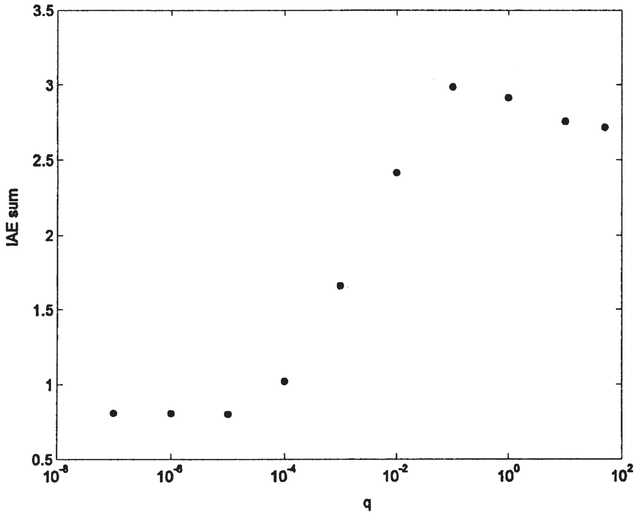


Figure 4. Change of IAE sum with respect to q.

where IAE_{RD} and IAE_{RB} are the performance scores in the estimation of the reflux-drum and the reboiler compositions, respectively. As a result, the optimum value of the considered design parameter is obtained from the simulation run giving the lowest sum of IAE_{RD} and IAE_{RB} values. The optimum value of the diagonal terms of process noise covariance matrix, q is searched in the range where the EKF estimator is stable. Performing some trial runs, the stability region of the estimator is found where the value of q is in the range of 50 and 1×10^{-7}. This region is searched by changing the value of q in 10 folds. For $r = 5000$, the change of IAE scores with q is given in Figure 4.

The diagonal terms of measurement model noise covariance matrix, r are changed between 0.5 and 5×10^{8} increasing in 10 folds and in each run, the diagonal terms of process noise covariance matrix, q is selected as 0.00001 which was previously determined as optimal. As in the case of q, the searching region for r is also determined by means of the stability concept. Figure 5 presents the relation of IAE sum with respect to r, graphically. The

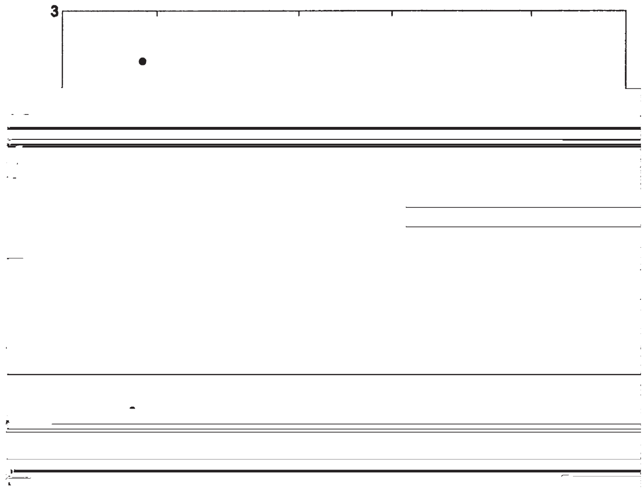


Figure 5. Change of IAE sum with respect to r.

best result (i.e., one having the lowest IAE sum) is obtained for the diagonal terms of process noise covariance matrix, = 5000 as shown in Figure 6.

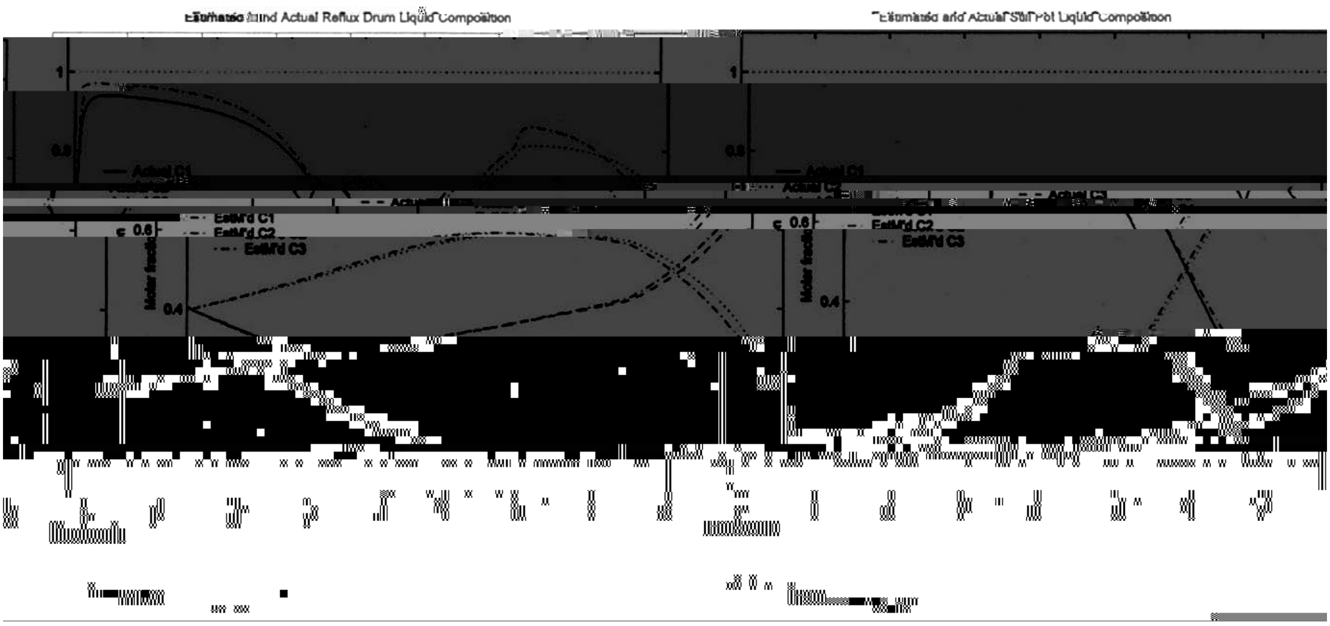
The previous runs were done, utilizing three measurement points for temperatures as stated by Quintero-Marmol (1991). Several extra runs with one to five measurement points were also conducted in which optimal values for the diagonal terms of process noise covariance matrix, and the diagonal terms of measurement model noise covariance matrix, are used, to see the effects of measurement points in EKF performance. Firstly, to decide on the number of measurement points, homogenously spreading the locations of the measurements throughout the column resulted in the IAE sums given in Table 8. The run having the lowest IAE sum is obtained as the one with three measurement points. In addition, the run with two measurements, which is the minimum number of measurements satisfying the observability criteria, has an IAE score, larger than that of the runs with more measurements and it has an IAE less than that of one-measurement run which is the only run violating column. The response for initial state estimate, $\underline{\ }_0 = [1/3; 1/3; 1/3]$ and the diagonal terms of its error covariance vector, $_0 = 0.1$ is shown in Figure 10. This is a fictitious composition for feed when the feed composition is not known. Of course, in this run the deviations in estimation are higher than the previous cases, giving IAE sum of 1.8797. However, they can still be considered agreeable in a case where feed composition is not known. Moreover, the estimations can also be improved with trial-and-error using different tuning parameters for the case of unknown feed composition.

In this phase of the study, it is aimed to analyse the performance of the EKF estimator for a MBDC system in a composition-feedback inferential control structure which realizes an actual scheduling policy explained previously in the section entitled MBDC Operation, where reflux-ratio is adjusted to a pre-optimized value with the use of top product composition information. In this control law, the compositions in the reflux-drum, the product-cut tanks and the reboiler are the inputs to the controller and the manipulated variable is the reflux-ratio of the column. The pre-specified reflux-ratio values required for the control algorithm is chosen as the optimized ones used in the previous sections. The tank, to which the distillate stream is diverted, and its timing are decided by monitoring the input compositions to the controller and utilizing the actual reflux-ratio policy. In the simulation of this control structure, the compositions can be obtained directly from the process simulation or from the EKF estimator. Firstly, to create a reference point, a simulation is done, taking the composition knowledge directly from the column as the feedback information to the controller. The desired product purities are the set points of the controller which are taken as 0.9, 0.81, 0.69. The response of this reference run in terms of the liquid compositions, both in the reflux-drum and the reboiler are given in Figure 11.

The capacity factor (CAP) (Luyben, 1988) and batch time (BT) are selected as the performanc(whe)-8(ned) asAP)(is(whe)-6

The closed-loop responses of the MBDC under the scheduling controller with actual composition feedback. (a) Reflux-drum compositions; (b) reboiler compositions.

affecting the performance of the EKF estimator is the selection of the VLE formulation. EKF parameters of the diagonal terms of process noise covariance matrix and the diagonal terms of measurement model noise covariance matrix are tuned in the range where the estimator is stable and selected basing on the least sum of individual IAE scores for the reflux-drum and the reboiler composition estimates. It is also found that, increasing the number of temperature measurements above the recommended value of NC does not result in a better performance. Although the observability criterion makes NC − 1 temperature measurements sufficient, using NC measurements improves the performance of EKF estimator. The measurement locations must be spread through out the column homogeneously for a better performance. Decreasing the measurement period value increases the estimator performance, and is limited by the computational power of the digital computer especially in real-time applications. The designed EKF estimator is successfully used in the composition—feedback inferential control of MBDC operated under variable reflux-ratio policy with an acceptable deviation of 0.5–3% from the desired purity level of the



The closed-loop responses of the MBDC under the scheduling controller with estimated composition feedback. (a) Reflux-drum compositions; (b) reboiler compositions.

products. The method proposed in the study utilizes a very simple model for EKF which is tested in a typical batch distillation column for estimation of states and which can also be utilized in continuous distillation columns easily.

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