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STATE ESTIMATOR DESIGN FOR MULTICOMPONENT BATCH DISTILLATION COLUMNS

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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, *n*-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.

Keywords: batch distillation; simulation; state observer; Kalman filter.

INTRODUCTION

'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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information about a system and state estimator is the tool responsible for gathering valuable measurements to infer the desired information. Modern estimators also use known relationships in computing the desired information; taking into account the measurement errors, the effects of disturbances and control actions on the system, and prior knowledge about the system and measuring devices. While gathering these elements, they make use of some error criteria and try to minimize errors in some respect. The criteria and the method of minimization characterize the method of estimation and the use of minimization makes the estimate (extracted information) 'optimal'. If this optimality is realized statistically, the estimator type becomes stochastic; if deterministically it becomes deterministic. The estimator used in this work falls in the stochastic category and it is named as Kalman filter.

In this study, the aim is to design a state estimator that infers the component concentrations of the multicomponent batch distillation column from the measured tray temperatures. The designed estimator is further tested using a rigorous column simulation to find its performance. The extended Kalman filter (EKF) is selected as the state estimator. In the literature, EKF has shown to provide good results in the chemical industry that includes model uncertainties, unmeasured process disturbances and noisy measurements. Because it is based on the linear dynamic model of the process, the rigorous model used in the simulation is adapted to the estimator algorithm mainly by simplifying the equilibrium model and by means of linearization. The performance of the developed estimator is tested by using the rigorous column simulation and discrete measurements of the top product compositions.

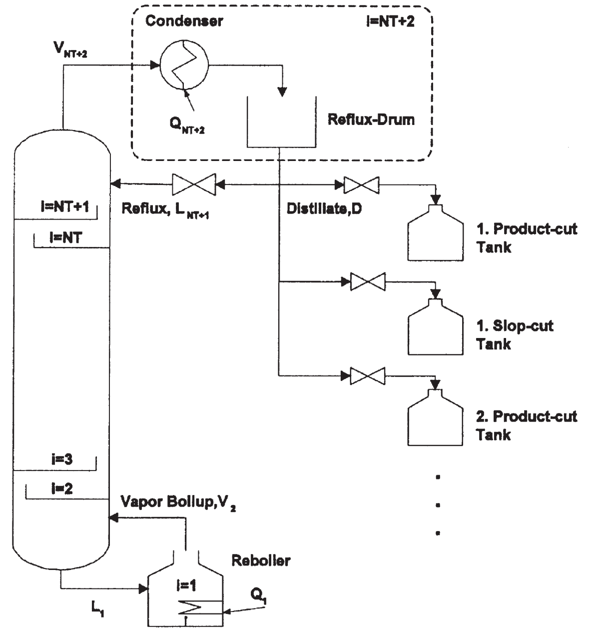

Figure 1. The schematic of a multicomponent batch distillation system.

MULTICOMPONENT BATCH DISTILLATION COLUMN (MBDC) OPERATION

In a batch distillation operation two types of products are handled (Luyben, 1988). The one named as slop-cut which is the byproduct of off-specification material and the other named as product-cut which is the product satisfying the specified purities. The operation of a batch column is divided into a number of stages as in the order of realization; start-up period, distillation at total-reflux, withdrawal of the lightest product, removal of a slop-cut, withdrawal of the next heaviest product, removal of a second slop-cut and, so on.

The operation for the MBDC given in Figure 1 is initiated by charging the feed mixture to the column, from its top, resulting in establishment of initial holdups in the order of condenser, reflux-drum, trays and reboiler. During this initialization period, no distillate is withdrawn from the column but instead the column is operated at total-reflux condition or at high reflux ratios to establish the desired purity level of the lightest compound in the reflux-drum. Then the first product-cut is started to distil by setting the reflux-ratio to a pre-specified value and in the same time the distillate stream is transferred to first product-cut storage tank. Due to the decreasing amount of the lightest compound in the column, after some time its composition level in the first product-cut tank begins to decrease. At this point, the distillate stream is diverted to the first slop-cut tank, if the composition of the next heaviest compound in the reflux-drum is below its specified purity. If however, it is not so low, or, during the slop-cut distillation, it starts to pass the specification level, then again the distillate is diverted to the second product-cut tank and the reflux-ratio is set to its new value. This cyclic operation between the product-cut and the slop-cut distillation continues until all the intermediate compounds is separated. Finally, the content of the reboiler is taken as the final product-cut which is rich in the heaviest compound.

MBDC PROCESS SIMULATION

There are many different rigorous models of batch distillation columns. They use the same basic strategy in the simulation model development which was used initially by the first studies on rigorous modelling of distillation columns. In batch column modelling, this common strategy was initiated by Meadows (1963) and Distefano (1968) which were followed by Stewart *et al.* (1973). In addition, the recent studies of Furlonge *et al.* (1999), Perry *et al.* (1999) and Venkateswarlu and Avantika (2001) can be given as the examples using this common strategy. The rigorous model used in this study is based on the study of Distefano (1968) and its details are given by Yıldız (2002). The assumptions employed in the development of the model can be found in Table 1, besides, Tables 2 and 3 summarize the rigorous model equations.

The assumption of negligible vapour holdup have been discussed by Young and Luyben (1987) and they stated, 'in columns operating at moderate pressures (less than 10 atm), this assumption is usually a good one'. In the study of Distefano (1968) on which the current simulation is based, the assumption of constant volume tray liquid holdup was discussed and it was realized that because of the severe variations in the tray compositions, assumption of constant molar or weight holdup is invalid in batch distillation calculations. Therefore using the constant-volume-holdup assumption will be employed in the model