

ROBUST DYNAMIC STATE ESTIMATION OF A BINARY DISTILLATION COLUMN

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Abstract: A nonlinear geometric observer is developed, which infers the distillate and residue compositions in a highly-nonlinear binary distillation column from temperature measurements. The estimator performance is evaluated by imposing severe step changes to the input variables. In particular, the capability of the observer reconstruction is assessed with regard to ill-conditioning of the observability matrix, initialisation of the composition estimates, and noise in the temperature measurements. *Copyright © 2004 IFAC*

Keywords: Distillation column; State estimation; Geometric observer

1. INTRODUCTION

The product composition estimation problem in distillation columns stems from the fact that composition measurements are often not available on-line, either because an on-line composition analyzer is itself not available, or because the delay associated with the composition measurements makes it impossible to use these measurements within a composition control loop.

Estimating the dynamic evolution of product composition profiles in continuous distillation is an issue that has attracted a number of researchers. Basically, all approaches consider using temperature (and possibly flow) measurements to reconstruct the product composition dynamics. A pioneering work in this field is that of Joseph and Brosilow (1978), who used a linear combination of temperature and flow measurements to estimate product composition in a multicomponent column. More recently, Yu and Luyben (1989) proposed a nonlinear estimator based on the classical Wang-Henke computation algorithm; the selection of the optimal temperature measurements to be fed to the estimator was made through singular value decomposition of the steady state matrix of gains between tray temperatures and manipulated variables. Mejdell and Skogestad (1991) developed a static partial-least-square (PLS) estimator using steady-state temperature data only; because PLS regression is a linear technique, nonlinearities between temperatures and

compositions were counteracted by using logarithmic transforms of these variables. Kano *et al.* (2000) proposed a dynamic PLS model where temperature, flow, heat duty and pressure data were regressed to provide product composition estimates; process dynamics was accounted for by including both current and past measurements into the input data set. Baratti *et al.* (1995) developed an extended Kalman filter using two tray temperature measurements to reconstruct the product composition dynamics in a pilot-plant column; they found that a critical issue in the reliability and robustness of the estimator is the tuning of the model error and measurement error covariance matrices.

Recently, Alvarez and Lopez (1999) proposed a nonlinear estimator based on the differential geometry theories. This method is principally characterized by its applicability to either observable or detectable systems, encompassing a broad class of plants in process system engineering. Furthermore, the proposed estimator design includes a robust local convergence and a systematic construction-tuning procedure. It was successfully applied to solve the local nonlinear estimation problem of a free-radical homopolymer reactor (Alvarez and Lopez, 1999; Alvarez, 2000), to infer the concentration in a catalytic reactor (Lopez *et al.*, 2002) and to monitor the pollutant concentration in an activated sludge process for wastewater treatment (Lopez *et al.*, 2004).

In this simulation work, a nonlinear geometric estimator is developed to provide on-line estimates of the dynamics of product compositions in a pilot-scale nonlinear binary distillation column using temperature and flow measurements. The estimator performance is discussed with respect to such issues as capability to reconstruct the system dynamics in response to severe inputs changes, and robustness with respect to composition profile initialization and noise in the temperature measurements.

2. THE PLANT MODEL

To avoid lengthy and expensive test runs on our pilot-scale distillation unit, the estimator performance is evaluated by using a detailed plant model as a surrogate of the real plant. The separation of a binary ethanol-water system at the atmospheric pressure is considered. It should be noted that this mixture exhibits a very marked nonideal thermodynamic behavior. As will be shown later, this provides a further challenge for the development of the estimator and may strongly impact its performance.

The model is a very reliable representation of a pilot-scale distillation unit equipped with thirty 300-mm sieve trays (tray spacing: 200 mm), a vertical thermosiphon reboiler, and a total shell-and-tube condenser. The average reflux drum and bottom holdups during normal operation are about 15 kg and 70 kg, respectively. The column is equipped with several Pt-100 probes to monitor on line the temperature profile on selected trays and on the bottom sump. Mass flow meters provide on-line measurements for the reflux rate, the distillate rate, the bottoms rate, and the feed rate. A vortex meter is used to measure the steam volumetric flowrate; the steam pressure and temperature are also measured on-line, so that a mass measurement is indirectly available for this stream. On-line composition measurements are not available, but liquid can be sampled and analyzed off-line by means of a gas chromatograph. All the measurements that are available on-line in the plant can be regarded as outputs that can be possibly made available to the estimator.

The plant dynamic model is based on the usual collection of material and energy balances, vapor-liquid equilibrium relationships, Murphree tray efficiency equations, and tray hydraulics correlations. In particular, the hydraulics of the liquid phase on the column trays is described by means of the nonlinear version of the Francis weir formula based on the actual tray geometry. The adjustable model parameters were kept to a minimum and were tuned by using the procedure outlined by Barolo *et al.* (2003). A very satisfactory match between simulated and experimental data was observed, both at steady state and in dynamic mode. In particular, temperature and composition profiles were reproduced very accurately, which is a crucial issue if the model has to be used to assess the performance

of a composition estimator. In the following, this detailed model will be referred to as “the plant”, against which the estimator performance is evaluated.

3. THE NONLINEAR ESTIMATOR

3.1 The simplified model

The nonlinear estimator is based on a simplified model of the plant, where the states simulated by the model are corrected by the available measurements. The main feature of the estimator is that it should be suited for on-line applications, hence the use of a simple model is to be preferred.

The simplified model (Baratti *et al.*, 1995) considers only the mass balance for one of the components of the binary system, while the energy balance on the trays is neglected by assuming that the vapor and liquid molar flows are constant in each section of the column. Following this assumption, the dynamics of the molar tray hold-ups is neglected. Tray holdup values are updated after an input variation by considering the steady-state values.

Vapor-liquid equilibria (VLE) at every stage are calculated by using the NRTL model for the estimation of activity coefficients, and assuming an ideal vapor phase. The Antoine equation is used to describe the vapor pressure as a function of temperature. The parameter values are reported in Gmehling and Onken (1977). Note that the parameters for the NRTL model and the vapor pressure equations are different from those used in the detailed model previously described. This mimics the fact that VLE cannot be described perfectly, an issue that may severely impact the estimator performance.

The composition y_j of the vapor phase leaving the generic j -th stage is calculated from the corresponding equilibrium value y_j^* by using the Murphree efficiency equation:

$$E_j = \frac{y_j - y_{j-1}}{y_j^* - y_{j-1}} \quad (1)$$

The efficiency was kept constant for all trays and was used as a tuning parameter to calibrate the steady state model, obtaining a value equal to 0.54 (this value is different from the one used in the detailed model). Finally, a linear pressure profile is assumed along the column, taking an overall pressure drop of 42 mmHg.

3.2 Estimator design

The nonlinear estimator developed to reconstruct the dynamics of the distillate and residue compositions is based on the differential geometry theory. A detailed discussion on the construction of the estimator can

be found in Alvarez and Lopez (1999). Only a brief summary of the procedure will be given here.

Let consider the nonlinear dynamics of the distillation unit, according to the following model representation:

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}, \mathbf{u}(t), \mathbf{r}), \quad \mathbf{x}(t_0) = \mathbf{x}_0, \quad \mathbf{x} \in \mathfrak{R}^n \\ \mathbf{y} &= \mathbf{h}(\mathbf{x}, \mathbf{r}), \quad \mathbf{y} \in \mathfrak{R}^m \end{aligned} \quad (2)$$

where \mathbf{x} are the states, \mathbf{u} are the inputs, \mathbf{r} are the parameters and \mathbf{y} are the measured outputs, that in this case are the two pilot tray temperatures.

According to Alvarez and Lopez (1999), the motion $\mathbf{x}(t)$ is detectable (i.e. partially observable) by means of the observability indexes k_1 and k_2 (where k_1 and k_2 are such as $k_1+k_2=k \leq n$) and the state partitions \mathbf{x}_I and \mathbf{x}_{II} (where \mathbf{x}_I are the observable states and \mathbf{x}_{II} are the unobservable states), if the following conditions are verified along the motion:

- the map $\Phi(\mathbf{x}, \mathbf{u}(t), \mathbf{r})$ is invertible;
- the unobservable dynamics \mathbf{x}_{II} , is stable.

The map Φ is given by:

$$\Phi(\mathbf{x}, \mathbf{u}(t), \mathbf{r}) = [h_1, \dots, L_f^{k_1-1} h_1, h_2, \dots, L_f^{k_2-1} h_2]^T \quad (3)$$

where $L_f^i h_j$ indicates the recursive directional derivative of the time-varying scalar field $h_j(\mathbf{x}, t)$, with $j=1, 2$ along with the time-varying vector-field $\mathbf{f}(\mathbf{x}, t)$.

Condition b) is satisfied, since the column is stable. Condition a) can be verified noting that the observability matrix \mathbf{Q} is equal to the Jacobian of Φ , that is:

$$\mathbf{Q} = \frac{\partial \Phi}{\partial \mathbf{x}_I} \quad (4)$$

Therefore condition a) is verified if the observability matrix has rank equal to $k=k_1+k_2$. If the above conditions are verified the following estimator can be constructed:

$$\begin{aligned} \dot{\hat{\mathbf{x}}}_I &= \mathbf{f}_I(\hat{\mathbf{x}}_I, \hat{\mathbf{x}}_{II}, \mathbf{u}(t), \mathbf{r}) + \mathbf{Q}^{-1} \mathbf{K}_0 [\mathbf{y} - \mathbf{h}(\hat{\mathbf{x}}_I, \mathbf{r})] \\ \dot{\hat{\mathbf{x}}}_{II} &= \mathbf{f}_{II}(\hat{\mathbf{x}}_I, \hat{\mathbf{x}}_{II}, \mathbf{u}(t), \mathbf{r}) \\ \hat{\mathbf{y}} &= \mathbf{h}(\hat{\mathbf{x}}_I, \mathbf{r}) \end{aligned} \quad (5)$$

where \mathbf{Q}^{-1} is the inverse of the observability matrix, and \mathbf{K}_0 is the constant gain matrix, whose entries are selected such as the error dynamics is stable (Alvarez and Lopez, 1999).

The first step to consider is the selection of the estimator structure, that is the dimension of the observable and unobservable state vectors. The selection is strictly related to the robustness of the estimator. Here, only two temperature measurements

are assumed to be available to the estimator; augmenting the dimension of the observable states leads to an increase of the Lie derivative order (see equation 3). This fact is detrimental to the robustness of the estimator and makes the correction algorithm highly complex from the algebraic point of view. It is worth noting that the VLE relationship between temperature and composition of the liquid phase is described by an implicit function, in which the NRTL model and the Antoine expression appear. The complexity of the map Φ , and then of the matrix \mathbf{Q} , grows as the order of the Lie derivative is increased. As result, the computational effort grows significantly.

In this work, several estimator structures were considered, each one obtained by changing the dimension of the observed state vector and the location of the two measured outputs. The results that have been obtained show that observing only two variables leads to the best compromise among efficiency, robustness and simplicity of the nonlinear estimator. In this case, the invertibility of the matrix Φ is satisfied if the observable state vector entries are the liquid compositions on the tray where the sensors are located. These states depend on temperature through the VLE relationships. Therefore:

$$\begin{aligned} \mathbf{Q} &= \begin{bmatrix} q_{11} & q_{12} \\ q_{21} & q_{22} \end{bmatrix}, \\ q_{11} &= \frac{dy_1}{dx_{I,1}}, \quad q_{12} = q_{21} = 0, \quad q_{22} = \frac{dy_2}{dx_{I,2}} \quad (6) \\ \text{Det}[\mathbf{Q}] &\neq 0 \end{aligned}$$

where $x_{I,1}$ and $x_{I,2}$ represent the entries of the observable state vector \mathbf{x}_I , i.e. the liquid composition on the trays where the temperatures y_1 and y_2 are measured.

No particular strategy was used to select the measurement sensor locations, because this aspect was not of interest to the present work, but it will be considered in the future. A heuristic approach based on consideration about the dynamic behavior of the system, as well as on some test runs carried out using different measurements locations, showed that the best choice is to use the temperature of the bottom and of the 22nd tray (the 23rd stage of the column numbering from the reboiler). In particular, the bottom of the column was selected because it has the largest inertia of the system, i.e. the slowest dynamics. On the other hand the 22th tray is a compromise between closeness to the top of the column, and robust observability.

The choices described above lead to the following estimator structure:

$$\begin{aligned}
k &= 2, \quad k_1 = 1 \text{ and } k_2 = 1 \\
\mathbf{x}_I &= [x_{I,1}, x_{I,2}]^T = [x_1, x_{23}]^T \\
\mathbf{x}_{II} &= [x_2, \dots, x_{22}, x_{24}, \dots, x_{32}]^T \\
\mathbf{y} &= [y_1, y_2]^T = [T_1, T_{23}]^T
\end{aligned} \tag{7}$$

where x_1 represents the ethanol mole fraction in the bottom, and x_{32} corresponds to the ethanol mole fraction in the distillate.

According to structure (6) it results:

$$\begin{aligned}
\Phi &= [T_1, T_{23}]^T \\
\mathcal{Q}^{-1} &= \begin{bmatrix} \left(\frac{dT_1}{dx_1}\right)^{-1} & 0 \\ 0 & \left(\frac{dT_{23}}{dx_{23}}\right)^{-1} \end{bmatrix}
\end{aligned} \tag{8}$$

The entries of the gain matrix \mathbf{K}_0 are the estimator tuning parameters. As proposed by Alvarez and Lopez (1999), they were selected as follows:

$$\mathbf{K}_0 = \begin{bmatrix} k_{11} & 0 \\ 0 & k_{22} \end{bmatrix} \quad \begin{aligned} k_{11} &= \omega_1 \\ k_{22} &= \omega_2 \end{aligned} \tag{9}$$

where ω_1 and ω_2 are the characteristic frequencies, which can be selected by considering the inherent dynamics of the column, that is by allowing the estimator response to be faster than the column one. It is worth noting that the gain matrix \mathbf{K}_0 is multiplied by the inverse of the observability matrix, whose entries are the inverse of the derivative of temperature with respect to the observed states. This derivative is almost zero when the ethanol concentration is close to the azeotrope point, leading to a difficult calibration of the estimator. This situation can occur on the 22nd tray, when a high purity in the distillate is required. The best compromise between efficiency and robustness of the estimator was obtained when $\omega_1=0.003$ and $\omega_2=0.01$.

4. RESULTS AND DISCUSSION

The estimator performance was evaluated by considering two different tests. The first one was a somewhat idealized situation, where the estimator was initialized correctly and the temperature measurements were noise-free. The second one was designed to assess the robustness of the estimator when the initial composition profile is not known exactly and temperature measurements are affected by noise.

The first experiment (Run 1) was mainly designed to evaluate the estimator structure, that is the dimension of the observability state vector and the location of measurement sensors. In this case the filter was initialized correctly by calculating the initial

composition profile through the simplified model, and assuming that all the input variables were known exactly. Furthermore, the temperature measurements were not affected by noise. This experiment was conducted in several steps, which are summarized in Table 1.

In all the step tests, the feed temperature was kept constant at 295.3 K and the bottom pressure was equal to 801 mmHg.

Table 1. Operating conditions of the first test (Run 1)

Time (min)	Feed flowrate (kg/h)	Feed ethanol mole fraction	Reflux flowrate (kg/h)	Steam flowrate (kg/h)
0	125	0.143	107.4	90.0
100	125	0.143	161.0	90.0
300	125	0.143	107.4	90.0
500	125	0.143	107.4	67.5
700	125	0.143	107.4	90.0
900	162.5	0.143	107.4	90.0
1100	125	0.143	107.4	90.0
1300	125	0.186	107.4	90.0

The results related to Run 1 are shown in Figures 1a and 1b, where the ethanol mole fraction in the distillate stream and in the residue as estimated through the nonlinear geometric observer are compared to the relevant composition profiles in the plant. In the Figures, also the ethanol mole fraction calculated through the simplified model is reported, in order to show how the nonlinear geometric observer improves the estimation results. In particular, for both the top and the bottom products the geometric observer corrects the simplified model dynamics by improving the speed of response to the input changes. In fact, the results show that the simplified model exhibits a slower dynamics with respect to the actual one.

The nonlinear estimator reconstructs the bottom composition profile with a great accuracy (Figure 1b), except when a step change in the feed composition is imposed to the system ($t = 1300$ min). In this case the correction is less efficient and there is an offset at the new steady state condition. It is worth noting that in this situation the simplified model is not able to reconstruct the bottom composition dynamics at all. Note that the feed composition is not a measured input; hence its updated value was not fed either to the estimator or the simplified model.

Different results are obtained for the reconstruction of the distillate composition (Figure 1a). Although the nonlinear observer properly corrects the dynamics of the simplified model, offsets at the new steady states occur for all the step changes imposed, except when the feed flowrate is varied ($t = 900$ min). This behavior is related to the value of the derivative of the temperature with respect to the liquid composition on the 22nd tray. This derivative decreases by two orders of magnitude when the

liquid composition on this tray varies from 0.135 to 0.85 mole fraction, leading to an increase of the correction term, that results in a excessive contribute of the latter with respect to the model term (see equations 5). A tuning parameter ω_2 smaller by two orders of magnitude would improve results at steady state, but with an unfavorable effect on the speed of response, making the estimator less prompt. Anyway, it is worth noting that the relative estimation error is always less than 1.3 %, and this value is within the experimental error of the liquid composition analysis. Furthermore, the ethanol mole fraction in the liquid phase at equilibrium is 0.88, when temperature is equal to 78.009 °C and pressure is kept constant at 750 mmHg (nominal condition on the 30th tray). When temperature is varied to 78.015 °C, the ethanol mole fraction at equilibrium becomes equal to 0.87. The temperature difference is much lower than the precision of the experimental measurement sensors; hence, requiring a higher precision in the distillate composition estimation is meaningless. Nevertheless, it is important to stress that the largest offset appears when the feed composition is changed ($t = 1300$ min), because the new feed composition is not updated to the estimator. Also in this case, the estimator significantly improves the simplified model composition profiles reconstruction.

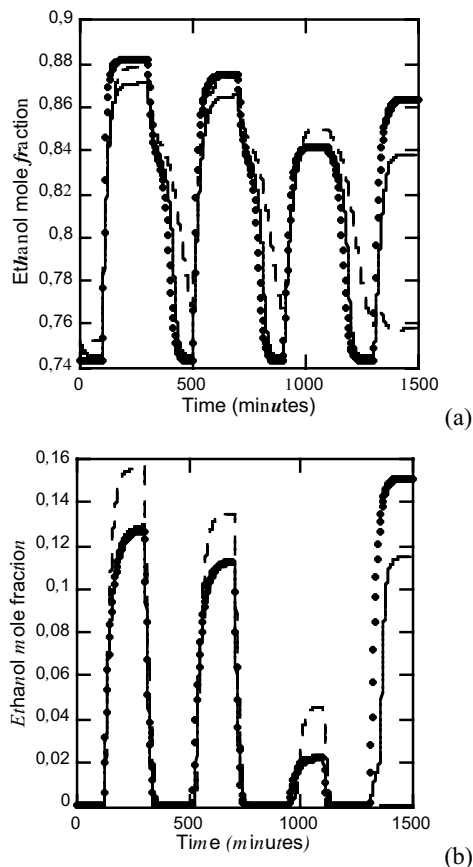


Figure 1. Comparison between plant (●), simplified model (dashed line) and estimated (solid line) ethanol mole fraction in the distillate (a) and residue (b) for Run 1.

The experiment described above deals with a somewhat idealized situation, because the temperature measurements were supposed to be noise-free and the estimator was initialized with a correct composition profile. In order to evaluate the robustness of the proposed nonlinear observer, a more demanding test was considered. In particular, the initial composition profile was calculated supposing that an incorrect feed composition (equal to 0.16 ethanol mole fraction) was available. Furthermore random numbers with zero mean and a standard deviation of 0.2 °C were superimposed to the temperature measurements in order to simulate noise.

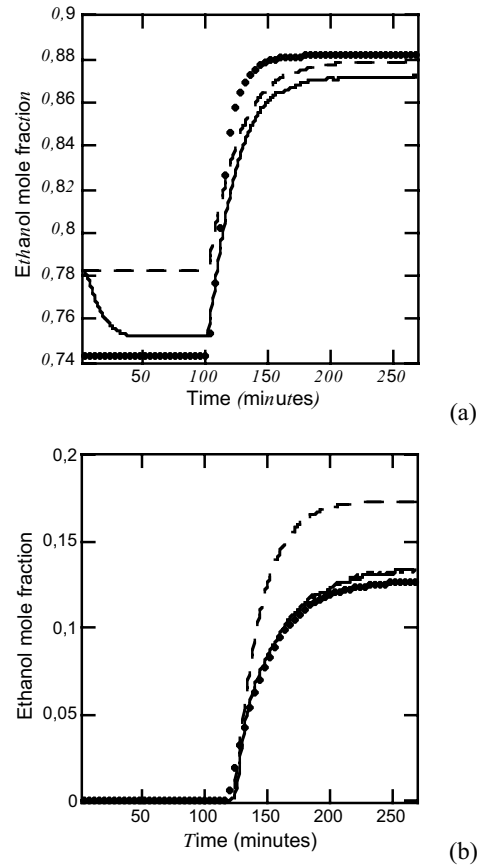


Figure 2. Comparison between plant (●), simplified model (dashed line) and estimated (solid line) ethanol mole fraction in the distillate (a) and residue (b) for Run 2.

The comparison between plant, simplified model and estimated ethanol mole fractions in the products are represented in Figures 2a and 2b, when a step change in the reflux flowrate from 107.4 to 161.0 kg/h is imposed to the system (Run 2). The results show that noise does not affect the estimator performance. This is mainly due to the low values of the constant gains k_{11} and k_{22} , which prevent that detrimental oscillations appear in the estimated composition profiles. On the other hand, the impact of the incorrect initialization is more evident. The estimator slowly corrects the initial states, reaching (in about 30 min) a new steady state value that differs from the exact one by ~ 0.003 (mole fraction). In this case the

small values of the tuning parameters have a negative effect on the initial speed of response; however, it is important to note that the offset is significantly reduced with respect to the simplified model predictions.

5. CONCLUSIONS

A nonlinear geometric observer was developed to estimate the distillate and bottom composition profiles in a highly nonlinear binary distillation column. The results were quite promising, although the structure of the correction algorithm led to adjust the estimator tuning parameters in a conservative way. This is mainly due to the structure of the correction term, based on the inverse of the observability matrix. This structure implies that the strength of the estimator correction term becomes excessive when the matrix determinant value is close to zero, that is when the ethanol concentration value is close to the azeotrope point. With a proper location of the measurement sensors, the estimator was tuned in such a way as to obtain a good compromise between efficiency and robustness. The estimator correction term was somewhat ineffective when the ethanol concentration in the feed was changed. However, it was evident that the estimator greatly improved the results when compared to the simplified model.

Nevertheless, the conservative tuning also implied positive effects; in fact the estimator performance was not affected by measurement noise. Furthermore, the selected calibration allowed to reduce the offset between the actual and the estimated ethanol concentration in the distillate in response to the input changes, allowing the estimator to provide composition estimates within the expected experimental error.

The presented results are the outcomes of a preliminary study on the development of a geometric observer for a simulated distillation process, and further investigations have been already planned in order to complete the survey. In particular, future work will be addressed on developing a strategy to select measurement location as well as on the compensation of estimator bias, when it exists. Furthermore, the estimator performance will be tested on the real pilot plant.

ACKNOWLEDGMENT. The authors acknowledge MIUR (grant 2002095147, PRIN 2002) for the financial support, and Prof. Jesus Alvarez, who

contributed to the development of the present paper by sharing his knowledge and ideas on the geometric approach.

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