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GEOMETRIC ESTIMATION OF TERNARY DISTILLATION COLUMNS

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Abstract: The problem of estimating effluent compositions from temperature measurements in ternary distillation columns is addressed within a geometric estimation framework where the estimation structure and the algorithm are jointly designed. The employment of passive estimation structures and error propagation measures yields criteria to choose the sensor number and locations as well as the set of innovated states. The proposed approach is tested with experimental data from a 32-stage pilot column (tert-butanol-ethanol-water system). With 64 on-line dynamical equations and a straightforward tuning scheme, the proposed estimator yields the same behaviour than the one of an Extended Kalman Filter with 2144 equations and an optimization-based tuning procedure

Keywords: distillation column, ternary distillation, passive estimation, process estimation

1. INTRODUCTION

Distillation is an important separation process, and the development of effluent composition estimation schemes is motivated by the need to design or redesign processes to meet more stringent safety, efficiency and quality specifications. In particular, a temperature measurement-driven estimation scheme: (i) is motivated by the cost, reliability and delay drawbacks of composition measurement instruments, and (ii) can be applied to improve the supervisory, advisory or feedback control tasks. The distillation and control problems have been extensively tested with a diversity of techniques, the related state of the art can be seen elsewhere (Baratti *et al*., 1995; Baratti *et al*., 1998; Oisiovici and Cruz, 2000; Venkateswarlu and Avantika, 2001), and here it suffices to mention that the nonlinear extended Kalman filter (EKF): (i) is the most widely used estimation technique, (ii) has been successfully tested in continuous and batch system over a wide range of separations and operating conditions, (iii) has an implementation that requires the tuning of covariance via trial-and-error (Oisiovici and Cruz, 2000;Venkateswarlu and Avantika, 2001) or optimization-based (Baratti *et al*. 1995, Baratti *et al*.1998) searches, and the on-line integration of a set of auxiliary ordinary differential equations (ODEs) whose number grows rapidly with stage number of stages and components. Moreover, it is not clear how the EKF nonlinearity and complexity features can be reconciled with the linearity and simplicity of the majority of the industrial linear (MIMO, decentralized, or one way-decoupled) PI and (MIMO) model predictive control schemes. In principle, the on-line integration of the EKF Riccati equations can be circumvented by employing the nonlinear geometric (Luenberger-like) estimation approach (Alvarez and Lopez, 1999, Alvarez, 2000), and the same approach enables the consideration of the sensor locations and the innovated states as design degrees of freedom, as it can be seen in previous polymerization reactors (Lopez and Alvarez, 2004) and (fixed-sensor) binary distillation column (Tronci *et al*., 2005) estimation studies. In a distillation column, estimation structure means the sensor locations and the set of innovated states, or equivalently, of states whose dynamical model has (direct) measurement injection.

The above considerations motive the scope of the present work: the development of a joint structure (i.e., the sensor location and innovated states-algorithm (i.e., the dynamic data processor) estimation design for ternary distillation columns, with a favorable comparison with the EKF technique in the light of complexity, reliability and implementation-tuning effort considerations. Following the geometric estimation approach (Alvarez, 2000, Lopez and Alvarez 2004), a single-sensor passive structure is chosen on the basis of suitable error propagation measures in conjunction with estimator testing, and the adjustable-algorithm is designed according to a geometric technique, without auxiliary Riccati equations, and with the estimation

structure as design degree of freedom. The proposed approach is tested with experimental data drawn from a 32-stage pilot column with the ethanol- tertbutanol-water system, finding that a passivated estimator with one sensor, 65 ODEs, and a conventional-like tuning scheme yields the same behavior than an EKF with two-sensors, 2144 ODEs, and a tuning drawn from the adjustment of six parameters using off-line optimization.

2. ESTIMATION PROBLEM

Consider an N-stage two-measurement (one per section) *continuous ternary distillation column*, with: (i) molar feed flow F at light- intermediate component composition pair (c^1_F, c^2_F), (ii) bottoms B (or distillate D) effluent rate at composition c_0 (or c_D) of light component, (iii) reboiler heat injection at rate Q (proportional to the vapor flow rate V), and (iii) two measurements, one in the stripping section and one in the enriching section, at locations to be determined. From standard (liquid-vapor equilibrium at each stage, quasi steady-state hydraulics and enthalpy balance with equimolar flow) assumptions, the column behavior is described by the following nonlinear dynamical system (Baratti *et al*. 1995; Skogestad, 1997):

Stripping section ($1 \leq i \leq n_F$, k = 1, 2)

$$\dot{c}^k_i=[(R+F)\,\Delta^+c^k_i - V\Delta^-\nu_k(c^1_i,c^2_i)]/\eta^i(R+F) \quad (1a)$$

Feed tray (i = n_F, k = 1, 2)

$$\dot{c}^k_{n_F} =[R\Delta^+c^k_{n_F} -V\Delta^-\nu_k(c^1_{n_F},c^2_{n_F}) + F(c^k_F-c^k_{n_F})]/\eta^i(R+F) \quad (1b)$$

Enriching section ($n_F + 1 \leq i \leq N-1$, k = 1, 2)

$$\dot{c}^k_i = [R\Delta^+c^k_i - V\Delta^-\nu_k(c^1_i, c^2_i)]/\eta^i(R) \quad (1c)$$

Top Tray (i = N, k = 1, 2)

$$\dot{c}^k_N = [R\Delta^+c^k_N - V\Delta^-\nu_k(c^1_N, c^2_N)]/\eta^i(R) \quad (1d)$$

Measurements

$$y_s = T_s = \beta(c^1_s, c^2_s),\ s \in [1, n_F -1] \quad (1e)$$

$$y_e = T_e = \beta(c^1_e, c^2_e),\ e \in [n_F +1, N] \quad (1f)$$

where (k = 1, 2)

$c^1_i + c^2_i + c^3_i = 1$, $\quad \Delta^+c^k_i = c^k_{i+1} - c^k_i$

$\Delta^-\nu^k_i(c^1_i, c^2_i) := \nu^k_i(c^1_i, c^2_i) - \nu_k(c^1_{i-1}, c^2_{i-1})$

$\nu_1(c^1_{-1}, c^2_{-1}) = c^1_0$, $\nu_2(c^1_{-1}, c^2_{-1}) = c^2_0$

$c^1_{N+1} = c^1_D = \nu_1(c^1_N, c^2_N)$, $\quad c^2_{N+1} = c^2_D = \nu_2(c^1_N, c^2_N)$

where c^1_i and c^2_i are the component (molar fraction) compositions in the i-th stage (the third component composition is given by $c^3_i = 1 - c^1_i - c^2_i$), y_s (or y_e) is the measured value of the temperature T_s (or T_e) in the s(or e)-th stage (to be determined) of the stripping (enriching) section, ν_1 (or ν_2) is the nonlinear (liquid-vapor equilibrium) function that determines the i-th component composition in the vapour phase, β is the nonlinear bubble point function that yields the temperature, and η is the tray hydraulics function that sets the exit molar flow rate from the i-th stage.

Knowning that, with at least two sensors, a ternary column is completely locally observable about a steady-state, (Yu and Luyben, 1987; Quintero-Marmol et al., 1991) and that this assesement should be revised in the light of a nonlinear instantaneous observability framework (Alvarez et al., 1999, 2000, 2004), a comment on the consideration of a single-sensor is in order: in a way that is analogous to the design of robust controllers via backstepping (Krstic et al., 1995, Alvarez *et al*., 2004), in the geometric estimation approach one gives up the (possibly illconditioned) complete (nominal) observability structure, in order to favor robustness, diminish observability requirements, at the cost of more sluggish reconstruction rate. From this viewpoint, it makes sense to consider a (possibly with illconditioned complete observability property) ternary distillation column with a robustly detectable single-sensor structure. In this robust partial observability structure case, the estimator has two components, one with measurement innovation and one noninnovated.

Our *estimation problem* consists in jointly designing the estimation structure (i.e., the sensor locations and innovated state set) and the estimation algorithm (the dynamic data processor) for ternary distillation columns. In particular, we are interested in: (i) the developing an estimator design that compares favourably with the EKF, in terms of complexity, reliability and implementation-tuning effort considerations, and (ii) in testing the approach with experimental data.

Experimental run. The experimental data were generated by a pilot distillation column fed by a water-ethanol-tertbutanol mixture (located at University of Padova, Italy). The column has 30 sieve trays, a vertical thermosiphone reboiler, and a total shell-tube condenser (the overhead vapour is totally condensed and the reflux drum is open to the atmosphere). The feed enters the column in the 8-th stage (i.e., n_F = 8), and there are temperature measurements in nine stages (0, 4, 8, 12, 16, 18, 22, 26 and 30). The top and bottom pressures were 814 and 760 mmHg, respectively, a linear pressure drop was assumed, and the liquid feed temperature T_F = 299 K was lower than the one (T-n_F = 366 K) the feed tray. The reflux, feed and vapor rate were (R, F) = (3.486, 3.489)10^{-5}m^3/s and vapor boilup rate V = 1.437 gmol/s, the feed compositions were $c^E_{n_F} = 0.0979$ and $c^T_{n_F} = 0.0630$. The initial condition corresponded to a steady-state with higher vapor flowrate V = 1.437 gmol/s. In other words, the column transient was induced by a step decrease in V, to a value of 0.963 gmol/s. For three different times, the resulting temperature profiles, drawn form simulations, are shown in Figure 1, and the corresponding effluent

concentrations over time can be seen in subsequent figures. Henceforth, super index E (or T) in c_i^k denotes the species ethanol (or ter-butanol) in the i-th tray. Due to the presence of close-to-azeotropic compositions in the enriching section, the related temperature profile is rather flat, and some components are in small amount, and consequently, the estimation task in the enriching section should be considerably more difficult than in the stripping section.

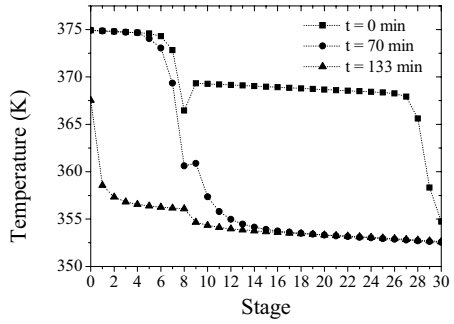

Figure 1: Simulated temperature profiles, at three different times.

3. PASSIVE ESTIMATION

From the adjustable-structure geometric estimation design (Alvarez, 2000; Lopez and Alvarez, 2004) in conjunction with the staged nature of the column, and the recent results of the method application to the binary case (Tronci *et al*. 2005), let us begin the structural assessment by considering single-sensor robustness-oriented *passive structures with one innovated state*. Further motivations for the employment of a passive estimation structure in a combined estimation-control passive design can bee seen elsewhere (Krstic *et al.,* 1995; Alvarez *et al*., 2004; Gonzalez and Alvarez, 2005; Alvarez *et al*., 2005).

3.1 Ethanol as single innovated state

Let us assume that a single sensor is located at the i-th column stage, and that the ethanol composition is the innovated state. The corresponding PI estimator is given by (Alvarez and Lopez, 1999):

$$\dot{\hat{c}}_i^E = f_i^E(\hat{c}_i^E, \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T) + [1/\beta_{c_E}(\hat{c}_i^E, \hat{c}_i^T)]\{\dot{w} + 2\zeta\omega[y_j - \beta(\hat{c}_i^E, \hat{c}_i^T)]\} \quad (2a)$$

$$\dot{w} = \omega^2[y_i - \beta(\hat{c}_i^E, \hat{c}_i^T)] \quad (2b)$$

$$\dot{\hat{c}}_i^T = f_i^T(\hat{c}_i^E, \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T), \quad k = E, T \quad (2c)$$

$$\dot{\hat{c}}_j^k = f_i^k(\hat{c}_j^E, \hat{c}_j^T, \hat{c}_{j-1}^E, \hat{c}_{j-1}^T, \hat{c}_{j+1}^E, \hat{c}_{j+1}^T), j \neq i, j \in [1,N] \quad (2d)$$

where

$$\beta_{c_E}(c_E, c_T) = \partial_{c_E}\beta(c_E, c_T), \quad S_i^E = 1/|\beta_{c_E}(c_i^E, c_i^T)| \quad (3a,b)$$

ω (or ζ) is the adjustable characteristic frequency (or damping factor) associated with the underlying nearly linear second-order output error dynamics, w is a dynamical state that estimates and compensates the effect of modelling errors in the predicted output, or equivalently, eliminates the output error mismatch. Due to the almost linear output error dynamics that underlies the preceding estimator construction, the tuning of the pair (ω, ζ) can be performed according to conventional-like techniques and tuning guidelines for second-order linear filters (Alvarez and Lopez, 1999). Typically, ω is from 3-to-15 times larger (faster) than the natural frequency of the measurement response. S_i^E is the asymptotic error propagation measure (Lopez and Alvarez 2004), and will be occasionally referred to as sensitivity measure.

Figure 2 shows the sensitivity measure dependency on the spatial (stage) location, for three different times. As it can be seen in Figure 2: the sensitivity measure profile worsens with time, especially in the enriching section. As expected due to the presence of close-to-azeotropic compositions in the enriching section, that section exhibits more error propagation measure than the stripping section. By far, the column bottom stage is the one with the least error propagation, and the high values of S_i^E in the enriching section question the employment of a sensor in that section, especially towards the top. If a sensor in this section was to be tried, it should be placed in the middle of the section, as a compromise between robustness and closeness to the effluent compositions.

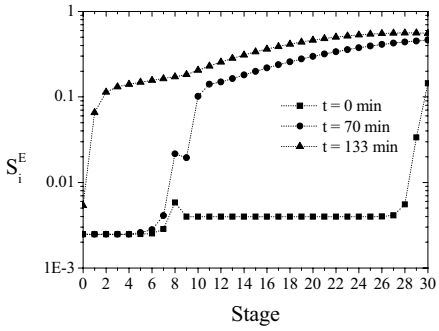

Figure 2: Singularity measure dependency on single-sensor location, when the ethanol composition is the innovated state, at three different times.

The straightforward application of conventional-like tuning guidelines (Alvarez and Lopez, 1999; Alvarez *et al*., 2004; Gonzalez and Alvarez, 2005) for second order linear filters yields the estimator parameters: ζ = 1.5 (to avoid oscillatory error response), ω = 0.03 min^{-1}. The resulting single-sensor (column bottom) estimator behavior is presented in Figure 3, showing that, as predicted by the sensitivity plot of Figure 2, the column bottom sensor exhibits a good data assimilation capability in the light of the uncertainty due to the composition off-line determinations. When the sensor is located in the middle of the enriching section, the bottom compositions estimates worsen, and there is not significant improvement in the distillate estimates. This corroborates the sensitivity measure-based prediction: a measurement in the enriching section hardly provides useful information.

Thus, according to Figure 3, the top effluent composition estimate task is basically being executed by the information content injected in the column bottom in conjunction with the column model.

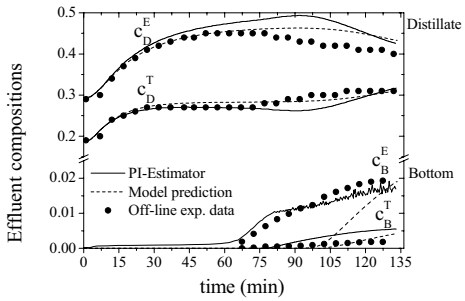

Figure 3. Single-sensor (column bottom) passive estimation (ethanol composition as innovated state).

3.2 Terbutanol as innovated state

When the terbutanol is the innovated state and the sensor in located at the (variable) i-th stage, the estimator (2) becomes:

$$\dot{\hat{c}}_i^T = f_i^T(\hat{c}_i^E, \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T) + \left[1/\beta_{c_T}(\hat{c}_i^E, \hat{c}_i^T)\right]\{\dot{w} + 2\zeta\omega[y_j - \beta(\hat{c}_i^E, \hat{c}_i^T)]\} \quad (4a)$$

$$\dot{w} = \omega^2[y_i - \beta(\hat{c}_i^E, \hat{c}_i^T)] \quad (4b)$$

$$\dot{\hat{c}}_i^E = f_i^E(\hat{c}_i^E, \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T), \quad k = E, T \quad (4c)$$

$$\dot{\hat{c}}_j^k = f_i^k(\hat{c}_j^E, \hat{c}_j^T, \hat{c}_{j-1}^E, \hat{c}_{j-1}^T, \hat{c}_{j+1}^E, \hat{c}_{j+1}^T), j \neq i, j \in [1,N] \quad (4d)$$

where

$\zeta = 1.5, \quad \omega = 0.03\ \text{min}^{-1}$

$\beta_{c_T}(c_E, c_T) = \partial_{c_T}\beta(c_E, c_T), \quad S_i^T = 1/|\beta_{c_T}(c_i^E, c_i^T)|$ (5a,b)

The corresponding asymptotic error propagation measure is presented in Figure 4.

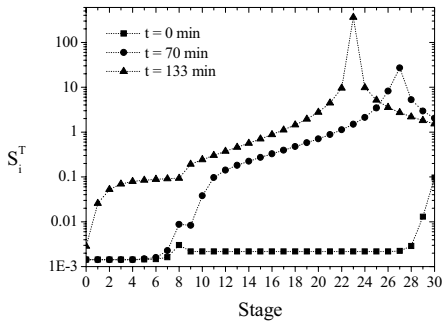

Figure 4. Singularity measure dependency on single-sensor location, when the terbutanol composition is the innovated state, at three different times.

According to Figure 4, the terbutanol should definitely not be chosen as the innovated state when the measurement is located about tray 23, and the same structure should not chosen for the stage interval 20-30. Comparing with Figure 2, when the measurement is located in the stage interval 0-16 either the ethanol or the terbutanol can be chosen as innovated state, and in both cases the location of sensors in the interval 20-30 should be avoided, especially for the case of terbutanol as innovated state. Physically speaking this means that: (i) in the stage interval 0-12 there is a sufficiently large temperature decrease for estimation purposes, with ethanol or terbutanol as innovated state, and (ii) in the stage interval 20-30 the estimation task via masurement injection is more difficult, could be pursued with the ethanol as innovated state but not with the terbutanol as innovated state, because the presence of ethanol (or terbutanol) is mildly (or imperceptible) reflected in the temperature measurement.

The resulting single-sensor (column bottom) estimator behavior is presented in Figure 5, with results that are similar to the ones of the case (Figure 3) with the ethanol as innovated state. Again, when the sensor is located in the middle of the enriching section, the bottom compositions estimates worsen, and there is not significant improvement in the distillate estimates.

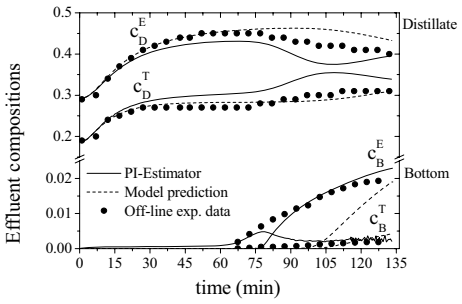

Figure 5. Single-sensor (column bottom) passive estimation (terbutanol composition as innovated state).

3.3 Concluding remarks

Being passivity originally an input-output control concept (Krstic *et al*., 1995), a comment on its interpretation in the estimation case is to the point. In out ternary distillation case, a passive estimation structure (2) [or (4)] signifies: (i) a single-state innovated dynamics, (i) a measured output-estimated input pair (y, w) with relative degree equal to one, and (iii) a stable (restricted) noninnovated dynamics (6) [or (7)]:

Ethanol as innovated state

$$\hat{c}_i^E = \gamma_E(\hat{c}_i^T, y_i) \quad (6a)$$

$$\dot{\hat{c}}_i^T = f_i^T[\gamma_E(\hat{c}_i^T, y_i), \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T], k = E, T \quad (6b)$$

$$\dot{\hat{c}}_j^k = f_i^k(\hat{c}_j^E, \hat{c}_j^T, \hat{c}_{j-1}^E, \hat{c}_{j-1}^T, \hat{c}_{j+1}^E, \hat{c}_{j+1}^T), j \neq i, j \in [1,N] \quad (6c)$$

Terbutanol as innovated state

$$\hat{c}_i^T = \gamma_T(\hat{c}_i^E, y_i) \quad (7a)$$

$$\dot{\hat{c}}_i^E = f_i^E[\gamma_E(\hat{c}_i^E, y_i), \hat{c}_i^T, \hat{c}_{i-1}^E, \hat{c}_{i-1}^T, \hat{c}_{i+1}^E, \hat{c}_{i+1}^T], k = E, T \quad (7b)$$

$$\dot{\hat{c}}_j^k = f_i^k(\hat{c}_j^E, \hat{c}_j^T, \hat{c}_{j-1}^E, \hat{c}_{j-1}^T, \hat{c}_{j+1}^E, \hat{c}_{j+1}^T), j \neq i, j \in [1,N] \quad (7c)$$

where γ_E (or γ_T) is the solution for c_E (or c_T) of the bubble point measurement equation $c_E = \gamma_E(c_T, y)$ [or $c_T = \gamma_T(c_E, y)$].

4. PASSIVATED ESTIMATOR

According to the constructive-like adjustable-estimation geometric estimation approach (Alvarez, 2000, Lopez and Alvarez 2004), the design of the estimation structure amounts to a suitable compromise between reconstruction rate and robustness, depending on the estimation objectives, the model conditioning of the particular system, and the measurement uncertainty. Low estimation degrees favour robustness and disfavour the reconstruction rate. In a general-purpose estimation structure search procedure [Lopez and Alvarez, 2004]: (i) the passive structure, with maximum robustness, must be seen as the point of departure candidate structure and configurations with more innovated states must be considered to draw the best compromise between robustness and performance, and (ii) the (nominal) detectability structure, with maximum estimation orders equal to the observability indices, constitutes the limit on performance in the absence of modelling errors. The particular (staged, three component, presence of azeotrops, and high separation) features of our ternary distillation column example suggest that the estimation structure should be more on the passive side, and the verification of this conjecture constitutes the scope of the present section.

4.1 Nonpassive structure

Let us recall that the column bottom stage offers the best means of effective data assimilation, the fact that ethanol and terbutanol perform equally well as single-innovated states, consider both the column bottom ethanol and terbutanol concentrations as innovated states with one sensor in the same stage, and write the corresponding PI estimator [Alvarez and Lopez, 1999]:

$$\dot{\hat{c}}_i = f_i(\hat{c}_i,\hat{c}_{i-1},\hat{c}_{i+1}, u) + O^{-1}(\hat{c}_i, \hat{c}_{i-1}, \hat{c}_{i+1}, u)[\pi w + k_p[y_j - \beta(\hat{c}_i)] \quad (8a)$$

$$\dot{w} = k_w[y_i - \beta(\hat{c}_i)], \quad \hat{c}_i = (\hat{c}^E_i, \hat{c}^T_i)' \quad (8b)$$

$$\dot{\hat{c}}^k_j = f^k_i(\hat{c}^E_j, \hat{c}^T_j, \hat{c}^E_{j-1}, \hat{c}^T_{j-1}, \hat{c}^E_{j+1}, \hat{c}^T_{j+1}, u), j \neq i, j \in [1,N] \quad (8c)$$

$$S^{E-T}_i = [1/msvO(c_i, c_{i-1}, c_{i+1}, u)] \quad (9)$$

where

$O(c_i, c_{i-1}, c_{i+1}, u) = \partial_{c_i}\phi(c_i, c_{i-1}, c_{i+1}, u), \quad \pi = (0,1)'$

$\phi(c_i, c_{i-1}, c_{i+1}, u) = \{\beta(c_i), [\partial_{c_i}\beta(c_i)]f_i(c_i,c_{i-1},c_{i+1}, u)\}'$

$k_p = (2\zeta + 1)(\omega, \omega^2)', \; k_w = \omega^3, \; u = (F, R, V, c_{iF})'$

O is the 2x2 observability matrix, S^{E-T}_i is the error propagation measure for a sensor located in the i-th stage, and msv means "the minimum singular value", and the corresponding plot is presented in Figure 6 (for three times).

Comparing with the same plots (Figures 2 and 4) of the passive structure cases, the two-innovated state error propagation measure is considerably larger, and this is due to: (i) the combination of interactions in O, (ii) the presence of first and second order partial derivatives of the equilibrium (ν_E and ν_T) and bubble point (β) nonlinear functions in O, (iii) stages with close-to-azeotropic compositions, and dependency of O on neighbour tray compositions. This results lead us to disregard nonpassive estimation structures.

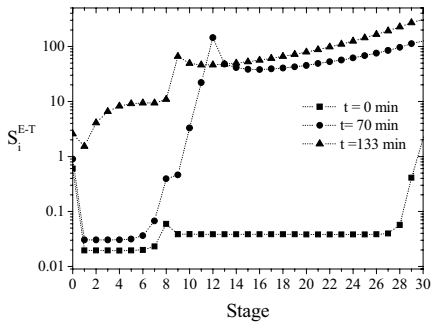

Figure. 6. Singularity measure dependency on (single) sensor location, when ethanol and tertbutanol are innovated state, at three different times.

4.2 Passivated structure

In a way that is analogous to the recursive robust control design via passivation (Krstic *et al*., 1995; Alvarez *et al.,* 2004), and motivated by the decentralized control design for distillation columns (Castellanos-Sahagun *et al*, 2005) as well as by the similar behavior of the passive structures with ethanol or terbutanol as innovated state, let us consider the parallel combination of the two passive estimators, (2) and (5), presented is Subsection 3:

$$\dot{\hat{c}}^E_i = f^E_i(\hat{c}^E_i, \hat{c}^T_i, \hat{c}^E_{i-1}, \hat{c}^T_{i-1}, \hat{c}^E_{i+1}, \hat{c}^T_{i+1}) + [1/\beta_{c_E}(\hat{c}^E_i, \hat{c}^T_i)]\{w_E + 2\zeta_E\omega_E[y_j - \beta(\hat{c}^E_i, \hat{c}^T_i)]\} \quad (10a)$$

$$\dot{w}_E = \omega^2_E[y_i - \beta(\hat{c}^E_i, \hat{c}^T_i)], \quad \dot{w}_T = \omega^2_T[y_i - \beta(\hat{c}^E_i, \hat{c}^T_i)] \quad (10b)$$

$$\dot{\hat{c}}^T_i = f^T_i(\hat{c}^E_i, \hat{c}^T_i, \hat{c}^E_{i-1}, \hat{c}^T_{i-1}, \hat{c}^E_{i+1}, \hat{c}^T_{i+1}) + [1/\beta_{c_T}(\hat{c}^E_i, \hat{c}^T_i)]\{w_E + 2\zeta_T\omega_T[y_j - \beta(\hat{c}^E_i, \hat{c}^T_i)]\} \quad (10c)$$

$$\dot{\hat{c}}^k_j = f^k_i(\hat{c}^E_j, \hat{c}^T_j, \hat{c}^E_{j-1}, \hat{c}^T_{j-1}, \hat{c}^E_{j+1}, \hat{c}^T_{j+1}), j \neq i, j \in [1,N] \quad (10d)$$

$\omega_E = \omega_T = 0.03$ min^{-1}, $\zeta_E = \zeta_T = 1.5$

Note that this estimator has a decentralized error propagation structure, with two passive error propagation mechanisms, one for each innovated state, that have been already displayed (in figures 3 and 5). Consequently, the (same) *sensor location assessment* of the passive cases is inherited by the preceding passivated estimator: (i) the column bottom stage is the best sensor location for bottom (and to a good extent also for distillate) composition estimation purposes, (ii) a sensor in the enriching section (say about tray 22) may be added, in the understanding that such addition may not bring in sufficiently meaningful information. The corresponding single-sensor (column bottom) behavior is presented in Figure 6 (discontinuous plots). Comparing with the two passive structures (Figures 3 and 5), the passivated structure yields a better behavior, or equivalently is a more efficient means to execute the data assimilation task.

4.4 Comparison with EKF

Here the proposed single-sensor passivated estimator is compared with an EKF with two sensors (in the reboiler and stage 27), as it is commonly done in distillation column studies. Since the EKF covariance matrix pair gain tuning is rather complex for the ternary case, the tuning procedure presented in an earlier study was followed (Baratti, et. al, 1995; Baratti, et. al, 1998): (i) a suitable structure of the model error covariance matrix was assumed, on the basis of the column sections and the number of components, (ii) and six matrix parameters were tuned using an optimization scheme. The resulting behavior is presented in Figure 7 (continuous plots), showing that basically the single-sensor passivated estimator (10) and the EKF yield the same behavior.

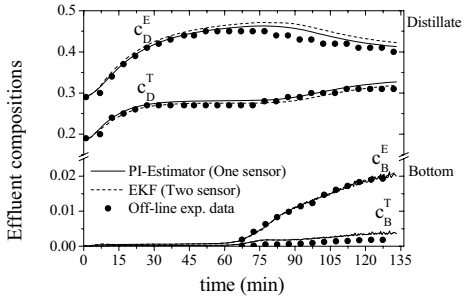

Figure 7. Comparison of the Single-sensor passivated PI-Estimador against the two-sensor EKF.

The advantage of the passivated estimator over the EKF resides in the fact that the construction, implementation and tuning tasks of the passivated are considerably simpler: (i) while the single-sensor passivated estimator has 65 nonlinear ODEs (64 for the model and one for the integral state), the EKF has 2144 nonlinear ODEs (64 for the model and 2080 Riccati equations), (ii) while adequate functioning of the EKF requires a nontrivial tuning via optimization, with parameters devoided of physical meaning, the passive estimator tuning can be performed according to conventional-like guidelines for linear second order filters, with (damping and frequency) parameters that have a clear connection with the column dynamics and the output prediction error response.

5. CONCLUSIONS

The problem of jointly designing the estimation structure and algorithm estimation to infer effluent compositions in ternary distillation columns with temperature measurements has been addressed and the results illustrated with a representative 32-stage experimental column. The constructive estimation approach associated with the adjustable-structure geometric estimation design methodology led to a single sensor (located in the column bottom) two-innovated state passivated estimator with 65 ODE's and a straightforward tuning scheme. The proposed estimator yielded the same behavior than the one obtained by a two-sensor EKF with 2144 nonlinear ODE's, and six tuning parameters chosen with an off-line optimization approach developed before.

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