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Measurement structure design for multicomponent distillation column with specific estimation objective

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Abstract: In this work, the problem of designing the estimation structure to infer some of the effluent compositions in a multicomponent distillation column is addressed, with the aim to determine the structure that yields the best estimator functioning in the sense of a suitable compromise between performance versus complexity, regardless of the particular estimation algorithm employed. The structure design involves the selection of (i) the number of modeled components, (ii) the innovated components, and (iii) the number and locations of sensors. The consideration of the problem within the adjustable-structure geometric estimation framework in the light of the column characteristics leads to a methodology with an analysis stage, where structures are screened and candidate ones are selected, followed by a synthesis stage which yields the structure with the best estimator functioning. The proposed approach is applied through simulations to an industrial-type hexacomponent distillation column, finding that the estimation task can be adequately performed with an algorithm whose number of ODEs (77) is considerably smaller than the one (2849) that results from the direct application of the standard EKF.

Keywords: multicomponent distillation column, estimation structure, geometric estimator

1. INTRODUCTION

Distillation is a typical energy intensive industrial operation where a stream is separated into two or more products, up to prespecified purities within given tolerances. The objective of the related control problem consists in efficiently performing the separation task in the presence of disturbances and has been extensively studied with conventional and advanced distillation techniques, including multicomponent separation (Venkateswarlu and Kumar (2006)) and reactive (Sundmacher and Kienle (2002)) distillation column cases. With the exception of the MIMO MPC (typically based on linear models), the majority of the industrial distillation column control schemes consist of sets of linear-decentralized conventional (P and PI) loops driven by temperature, composition or composition-temperature measurements. Even though the model-based nonlinear controllers implemented with nonlinear observers have provided valuable understanding and insight, the industrial implementation of the associated nonlinear dynamical and highly interactive control systems still raises serious complexity, reliability, and investment-maintenance cost concerns among control practitioners. Thus, at this point, the development of improved monitoring strategies for advisory or supervisory control purposes (to assist the adjustment of set-points in conventional-like industrial control schemes), constitutes a more realistic justification for the development of model-based nonlinear composition estimators for industrial multicomponent distillation columns. These considerations motivate the present estimation study.

The Extended Kalman Filter (EKF) (Jazwinsky (1970)) has been by far the most widely used estimation technique to infer compositions, on the basis of temperature measurements, in distillation columns, especially in the multicomponent case. Given the availability of adequate models (Skogestad (1997); Baratti et al. (1998)), the EKF has been successfully implemented in binary (Baratti et al. (1998); Yang and Lee (1997)), ternary (Baratti et al. (1998)), and four-component systems (Venkateswarlu and Kumar (2006)). The advantages of the EKF are: (i) the accumulated experience to set diagonal measurement and block diagonal modeling error covariance matrices (Baratti et al. (1998); Álvarez and Fernandez (2009)) which otherwise is in general a complex tuning task, (ii) the straightforward construction once the structure of the error covariances are known, and (iii) the robust functioning in the sense of functioning over an ample set of column (continuous, batch) types, conditions and separation mixtures. On the other hand, from an industrial perspective, the main disadvantages of the EKF are: (i) the number or ODE's which must be on-line integrated, in a number which grows rapidly with the number of stages and components, (ii) the complexity of the tuning scheme in the sense of

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the lack of a clear connection between the entries of the error covariance matrices and the observer convergence, (iii) the lack of formal stability-based convergence assessments, and (iv) the lack of systematic means to choose the measurement structure (number of sensors and their locations). Motivated by these limitations, the distillation column estimation problem has been addressed within the so-called Geometric Estimation (GE) framework (Álvarez (2000); Álvarez and Fernandez (2009)), where: (i) the estimation design is performed in the light of a specific estimation objective, (ii) the estimation structure is a key design degree of freedom, (iii) the on-line integration of Riccati equations is not needed, (iv) there is a robust convergence criterion coupled with simple (conventional-like) tuning guidelines, and (v) the GE and EKF are formally connected. By structure it is meant the choice of modeled states, the innovated states (i.e. states with direct measurement injection), the data assimilation versus error propagation scheme, and the number and kind of measurements. The adjustable-structure GE approach has been successfully tested with: (i) experimental binary (Tronci et al. (2005); Álvarez and Fernandez (2009)), and ternary columns (Pulis et al. (2006); Pulis (2007)), and (ii) a simulated industrial six-component continuous distillation column (Frau et al. (2009)). Hitherto, these studies have regarded the structure as design degree of freedom, but have not addressed the problem of finding the best structure with respect to functioning. This problem has recently been addressed for a binary distillation column with experimental data (Fernandéz (2009)) and the consideration of this problem for the multicomponent case in an industrial setting constitutes the subject of this study.

In this work our problem consists of designing the estimation structure to infer some of the effluent compositions in a multicomponent distillation column, with the aim to determine the structure which yields the best estimator functioning with respect to the estimation objective, in the sense of a suitable compromise between performance versus complexity, regardless of the particular estimation algorithm employed. Since in our previous work (Frau et al. (2009)) the structural aspect with emphasis on modeled states was addressed, now the attention is on: (i) the measurement structure, in sense of the selection of the number and location of sensors, and (ii) the innovated components, in sense of components with direct measurement injection. Here the functioning will be tested against thermodynamic and feed composition errors. The consideration of the problem within the adjustable-structure geometric estimation framework in the light of the column characteristics leads to a methodology with an analysis stage, where structures are screened and candidate ones are produced, followed by a synthesis stage which yields the structure with the best estimator functioning. The methodology applied in the present work is therefore tested with an industrial six-component C3-C4 splitter.

2. ESTIMATION PROBLEM

2.1 Structural problem

Consider a multicomponent distillation column with N stages and C components operating in continuous regime, say with a conventional single-point PI temperature controller: if standard assumptions (energy balance neglected on each tray, feed variations due to feed and reflux subcoolings only, tight controller and condenser level control and ideal vapor-liquid equilibrium) hold, therefore the dynamic column behavior is described by the following model (Skogestad (1997); Baratti et al. (1998)):

Reboiler ($i = 1$, $j = \rho_1, \ldots, \rho_{C-1}$)

$$\dot{c}_1^j = \frac{R_S(c_2^j - c_1^j) - V_S v_1^j}{M_1} = f_1^j(\mathbf{c}_1, c_2^j) \tag{1a}$$

Stripping section ($2 \leq i \leq N_F - 1$, $j = \rho_1, \ldots, \rho_{C-1}$)

$$\begin{aligned} \dot{c}_i^j &= \frac{R_S(c_{i+1}^j - c_i^j) - V_S(v_i^j - v_{i-1}^j)}{M_i} \\ &= f_i^j(\mathbf{c}_{i-1}, \mathbf{c}_i, c_{i+1}^j) \end{aligned} \tag{1b}$$

Feed tray ($i = N_F$, $j = \rho_1, \ldots, \rho_{C-1}$)

$$\begin{aligned} \dot{c}_{N_F}^j &= \frac{R_E c_{N_F+1}^j - R_S c_{N_F}^j - V_E v_{N_F}^j + V_S v_{N_F-1}^j}{M_{N_F}} \\ &= f_{N_F}^j(\mathbf{c}_{N_F-1}, \mathbf{c}_{N_F}, c_{N_F+1}^j) \end{aligned} \tag{1c}$$

Enriching section ($N_F - 1 \leq i \leq N - 2$, $j = \rho_1, \ldots, \rho_{C-1}$)

$$\begin{aligned} \dot{c}_i^j &= \frac{R_E(c_{i+1}^j - c_i^j) - V_E(v_i^j - v_{i-1}^j)}{M_i} \\ &= f_i^j(\mathbf{c}_{i-1}, \mathbf{c}_i, c_{i+1}^j) \end{aligned} \tag{1d}$$

Top tray ($i = N - 1$, $j = \rho_1, \ldots, \rho_{C-1}$)

$$\begin{aligned} \dot{c}_i^j &= \frac{R_T c_N^j - R_E c_{N-1}^j - V_T v_{N-1}^j + V_E v_{N-2}^j}{M_{N-1}} \\ &= f_i^j(\mathbf{c}_{N-2}, \mathbf{c}_{N-1}, c_N^j) \end{aligned} \tag{1e}$$

Condenser ($i = N$, $j = \rho_1, \ldots, \rho_{C-1}$)

$$\dot{c}_N^j = \frac{V_T v_{N-1}^j - R_T c_N^j}{M_N} = f_N^j(\mathbf{c}_{N-1}, c_N^j) \tag{1f}$$

Temperature measurements ($i = 1, \ldots, m$)

$$T_{s_i} = \beta(\mathbf{c}_{s_i}, P_{s_i}) \tag{1g}$$

where $v_i^j = \epsilon_j(\mathbf{c}_i, P_i)$, $\mathbf{c}_i = [c_i^{\rho_1}, \ldots, c_i^{\rho_{C-1}}]^T$, and $\mathbf{c}_F = [c_F^{\rho_1}, \ldots, c_F^{\rho_{C-1}}]^T$. In the notation above, ρ_j is the name of the j-th component, m is the number of sensors along the column and s_i is the location of the i-th sensor, $c_i^{\rho_j}$ and $v_i^{\rho_j}$ are respectively the liquid and the vapor composition of the j-th component at i-th stage, $\mathbf{c}_i$ is the liquid composition vector at i-th stage, T_{s_i} is the temperature at s_i-th stage, P_i is the pressure at i-th stage, F is the feed flow rate with composition $\mathbf{c}_F$, R_S, R_E, R_T and V_S, V_E, V_T are respectively the liquid and vapor flows in the stripping section, enriching section and top tray, M_i is the holdup at i-th stage, β is the bubble-point implicit function that sets the temperature. The components $c_i^{\rho_C}$ for $i = 1, \ldots, N$ are determined by the (mass conservation) condition $\sum_{j=1}^{C} c_i^{\rho_j} = 1$.

In a typical industrial situation one is interested in drawing estimates of some key components within a given estimation error tolerance, determined by: (i) the measurement error uncertainty of the effluent composition determinations which are occasionally offline performed for monitoring and advisory temperature control purposes, (ii)

the admissible compositions variability of the automatic feedback control scheme, and (iii) the present versus target variability of the column operation over an extended time horizon. Thus, the estimator behavior should be judged not only by the performance against the actual model or measured compositions, but above all against the instrument uncertainty, admissible variability of the controller, and inherent plant variability.

The estimation problem consists in jointly designing the *estimation structure* (meaning the number of modeled components, the innovated components, and the number and locations of sensors) and *algorithm* (dynamic data processor) to infer some effluent compositions, in the light of a pertinent *estimation objective*, to obtain the best estimator functioning according to a suitable compromise between performance, robustness and simplicity. The Geometric Estimator (GE) provides a systematic tuning-construction over all admissible structures, and therefore has been chosen as estimation algorithm. Here the focus is on the choice of the robustness-oriented passive estimation structure.

In what follows, the structure estimation problem is technically formulated. Consider the compact notation for actual column dynamics given in (1):

$$\dot{x}_P = f_P(x_P, u_P, d_P) \qquad y_P = h_P(x_P) \tag{2}$$

where $x_P = [\mathbf{c}_1{}^T, \ldots, \mathbf{c}_N{}^T]^T$, $u_P = [R_T, V_S]^T$, $d_P = [F, c_F{}^T]^T$, $y_P = [T_{s_1}, \ldots, T_{s_m}]^T$, and $\dim(x_P) = n = N(C-1)$. In (2) x_P, u_P, d_P and y_P are respectively the states, the inputs, the disturbances and the outputs of the actual system.

The specialization to the multicomponent distillation case of the definition of robustness-oriented passive GE structure is formally described as follows:

$$\sigma = \{M, s, \mu\} \qquad M = \{\rho_{M_1}, \ldots, \rho_{M_{C_M}}\} \tag{3}$$
$$\mathbf{s} = [s_1 \ldots s_m]^T \qquad \mu = \{\mu_1, \ldots, \mu_m\}$$

where $C_M \leq C$, $m \leq N$, $\rho_{M_i} \in \rho = \{\rho_1, \ldots, \rho_C\}$, $1 < s_i < N$ and $\mu_i \in M$.

In the notation above, C_M and M are respectively the number and the set of modeled components, ρ is the actual component set, ρ_{M_i} is the name of the i-th modeled component, m is the number of sensors, s_i and μ_i are respectively the i-th sensor location and the innovated component at s_i-th stage.

Thus, the corresponding C_M-component estimator model associated with (1), in compact notation is given by:

$$\dot{x} = f(x, u, d) \qquad y = h(x) \tag{4}$$

where $x = [\mathbf{c}_1{}^T, \ldots, \mathbf{c}_N{}^T]^T$, $u = [R_T, V_S]^T$, $d = [F, c_F{}^T]^T$, $y = [\beta_{M_{s_1}}, \ldots, \beta_{M_{sm}}]$, $\mathbf{c}_i = [c_i^{\rho_1}, \ldots, c_i^{\rho_{C_M-1}}]^T$, $\mathbf{c}_F = [c_F^{\rho_1}, \ldots, c_F^{\rho_{C_M-1}}]^T$, $\beta_{M_{s_i}} = \beta_M(\mathbf{c}_{s_i}, P_{s_i})$ and $\dim(x) = n_M = N(C_M - 1) \leq n$.

In (4) x, u and d are respectively the model states, input and disturbances, $\mathbf{c}_i$ is the model vector composition at i-th stage, $\mathbf{c}_F$ is the model vector feed composition and $\beta_{M_{s_i}}$ is the model bubble-point function.

The estimation model (possibly with reduced number of components) is an important design degree of freedom. Based on this model, the corresponding adjustable-structure proportional integral (PI) GE with passive structure (Álvarez (2000); Álvarez and Fernandez (2009)) is given by:

$$\dot{\hat{x}}_I = f_I(\hat{x}, \hat{u}, \hat{d}) + \Phi(K_P(y_P - \hat{y}) + z) \tag{5}$$
$$\dot{\hat{x}}_{II} = f_{II}(\hat{x}, \hat{u}, \hat{d}) \qquad \dot{z} = K_I(y_P - \hat{y}) \qquad y = h(x)$$

where $\hat{x} = [\hat{x}_I^T, \hat{x}_{II}^T]^T$, $f = [f_I{}^T f_{II}{}^T]^T$, $x_I = [c_{s_1}^{\mu_1}, \ldots, c_{s_m}^{\mu_m}]^T$, $\dim(x_I, x_{II}) = (m, n_M - m)$, $\Phi = \mathrm{diag}(\frac{1}{\beta_{c_{s_1}^{\mu_1}}}, \ldots, \frac{1}{\beta_{c_{sm}^{\mu_m}}})$, $\beta_{c_{s_m}^{\mu_m}} = \left.\frac{\partial \beta_{M_{s_i}}}{\partial c_{s_i}^{\mu_i}}\right|_{\hat{\mathbf{c}}_{s_i}}$, $K_P = \mathrm{diag}(2\xi_1\omega_1, \ldots, 2\xi_m\omega_m)$, and $K_I = \mathrm{diag}({\omega_1}^2, \ldots, {\omega_m}^2)$.

In the notation above, $\hat{x}$, $\hat{u}$, $\hat{d}$, and $\hat{y}$ are the estimates of x, u, d and y. x_I and x_{II} are the innovated and non-innovated state sets. The estimator has $n_M + m$ states. The proportional and integral gain matrices K_P and K_I have been chosen according to the tuning guidelines (Álvarez (2000)). ω_i and ξ_i are respectively the characteristic frequency and the damping factor of the estimator at s_i-th stage. The characteristic frequency ω_i must be chosen between 5 and 10 times faster than ω_{o_i} (natural temperature characteristic frequency at s_i-th stage).

Thus, our problem consists in choosing the estimation GE-structure which yields the best estimator functioning with respect to a specific estimation objective, with functioning meaning suitable compromise between reconstruction speed and robustness.

2.2 Case example

Consider the industrial 37-stage hexacomponent distillation column (T110) located at SARAS refinery (Sarroch, Italy). The column is a C3-C4 splitter fed, at 19-th stage, with significant concentrations of propane (C3), iso-butane (IC4) and n-butane (NC4) (primary components) as well as ethane (C2), iso-pentane (IC5) and n-pentane (NC5) in small amounts (secondary components). The column has a kettle reboiler (1-st stage), and a total condenser (37-th stage). The pressure changes linearly along the column from 16.3 Kg·cm^{-2} to 16.6 Kg·cm^{-2}. The column has a PI temperature controller which manipulates the heat injection rate (proportional to the vapor flow V_S leaving the reboiler) on the basis of the temperature at the 28-th stage, according to standard Ziegler-Nichols tuning rules (with $K_C = 10$ and $\tau_I = 0.6$). It must be pointed out that this example represents a typical industrial situation, where some of the primary components must be split in the presence of secondary components.

Under standard assumptions, the 6-component column dynamics are given by (1) with $N = 37$, and $C = 6$. The thermodynamics (liquid-vapor equilibrium and bubble point functions) are set with the (7-parameter) Extended Antoine equation (constants taken from ASPEN database).

The *estimation objective* is the inference of the distillate IC4 and bottom C3 composition within the 10% relative error (referred to nominal values). This percentage is determined by the admissible control variability for the component ($\approx 25\%$) and by the uncertainty of the discrete-delayed experimental concentration determinations per-

formed for product-process monitoring and quality supervisory control purposes. Thus, our problem consists in choosing the particular GE structure (3) where

$$\begin{array}{l} \rho_{M_i} \in \rho = \{C2, C3, IC4, NC4, IC5, NC5\} \\ C_M \leq 6 \qquad m \leq 37 \qquad 1 \leq s_i \leq 37 \end{array} \tag{6}$$

which yields the best estimator functioning as a suitable compromise between simplicity, reconstruction speed, and robustness (with respect to thermodynamics approximation and unknown feed composition errors).

In our previous work (Frau et al. (2009)), having as a point of departure the actual component set ρ given in (6), the problem of choosing the modeled states has been addressed and solved for the given column by choosing $M = \{C3, IC4, NC4\}$. Thus, our present problem amounts to determining the measurement structure s and the innovated component set μ. In this work, the best estimator functioning is assessed when thermodynamic and feed composition errors are present.

3. STRUCTURE SEARCH

In a previous study (Frau et al. (2009)), the set $M = \{C3, IC4, NC4\}$ of modeled components has been determined from the steady-state temperature gradient versus stage diagram (including per-component contributions), on the basis of the detailed 6-component model (2). In other words, $\{C2, IC5, NC5\}$ is the set of unmodeled components. Consequently, the resulting *estimation model* is given by (4) with $C_M = 3$, $N = 37$, and $n_M = 74$.

The actual system (2) and estimator model (4) were set about the SS with reflux $R_T = 75.7$ m^{3}h^{-1}, vapor $R_T = 1257.1$ m^{3}h^{-1}, feed flow $F = 66$ m^{3}h^{-1} and composition values listed in Table 1. The unmeasured estimator feed concentration will be set constant at its nominal value, listed in Table 1. The estimator model (4) is set with an Antoine equation-based approximation (Reid et al. (1998)) of the actual thermodynamics, based on an Extended Antoine equation. The corresponding SS composition profiles are presented in Figure 1 showing that: (i) the actual and modeled C3 bottom compositions are rather similar (about 10^{-6}% error difference); (ii) the actual and modeled IC4 distillate compositions are rather different (about 13% error difference). This behavior comparison exhibits what the estimator asymptotic behavior should achieve: the reduction of the distillate IC4 composition error, while maintaining the bottom C3 composition error small.

Table 1. Feed composition (molar fractions) for 6-component system (2) and 3-component model (4)

	6-component system	3-component model
C2	0.001	
C3	0.324	0.281
IC4	0.257	0.236
NC4	0.4042	0.483
IC4	0.004	
NC5	0.0008	

3.1 Structural analysis

Motivated by the GE detectability measures (López and Álvarez (2004); Fernandéz (2009)) employed in previous

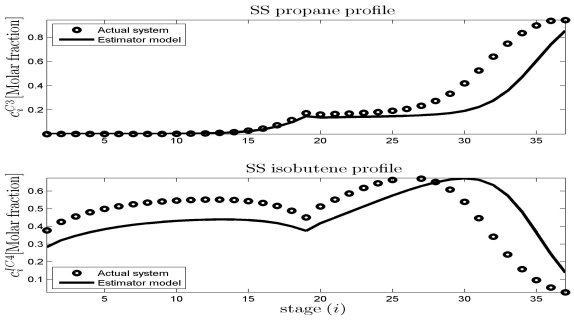

Fig. 1. SS composition profiles for 6-component system (2) (black circles) and 3-component estimator model (4) (black line)

binary (Tronci et al. (2005); Fernandez and Álvarez (2007); Álvarez and Fernandez (2009); Fernandéz (2009)) and ternary columns (Pulis et al. (2006); Pulis (2007)), and by the SS stage-to-stage temperature gradient diagram (with per-component contributions) employed to reduce the number of components in the model (Frau et al. (2009)), in this section the diagram is: (i) connected with the asymptotic error propagation measure (Fernandéz (2009)) and (ii) used to draw a set Σ of candidate structures.

In detailed form, the GE σ-structure (5) is written as:

Innovated components ($i = 1, \ldots, m$):

$$\dot{\hat{c}}^{\mu_i}_{s_i} = \hat{f}^{\mu_i}_{s_i}(\hat{\mathbf{c}}_{s_{i-1}}, \hat{\mathbf{c}}_{s_i}, \hat{c}^{\mu_i}_{s_{i+1}}) + \frac{1}{\beta_{c^{\mu_i}_{s_i}}} \left(2\xi_i \omega_i (\tilde{T}_{s_i} - \tilde{y}_{s_i}) + z_{s_i} \right) \tag{7a}$$

$$\dot{z}_{s_i} = {\omega_i}^2 (\tilde{T}_{s_i} - \tilde{y}_{s_i})$$

Noninnovated components($\{\rho_j, k\} \neq \{s_i, \mu_i\}$)

$$\dot{\hat{c}}^{\rho_j}_k = \hat{f}^{\rho_j}_k (\hat{\mathbf{c}}_{k-1}, \hat{\mathbf{c}}_k, \hat{c}^{\rho_j}_{k+1}) \tag{7b}$$

where $\tilde{T}_{s_i} = T_{s_i} - \beta_{M_{s_i}}$ and $\tilde{y}_{s_i}$ takes into account temperature thermodynamic and measurement errors at s_i-th stage.

The corresponding estimation error dynamics are:

Innovated components ($i = 1, \ldots, m$):

$$\dot{\tilde{c}}^{\mu_i}_{s_i} = \tilde{f}^{\mu_i}_{s_i} + \frac{1}{\beta_{c^{\mu_i}_{s_i}}} \left(2\xi_i \omega_i (\tilde{T}_{s_i} - \tilde{y}_{s_i}) + {\omega_i}^2 \int (\tilde{T}_{s_i} - \tilde{y}_{s_i}) \right) \tag{8a}$$

$$\approx \tilde{f}^{\mu_i}_{s_i} + 2\xi_i \omega_i \tilde{c}^{\mu_i}_{s_i} + {\omega_i}^2 \int \tilde{c}^{\mu_i}_{s_i} - \frac{2\xi_i \omega_i \tilde{y}_{s_i} + {\omega_i}^2 \int \tilde{y}_{s_i}}{\beta_{c^{\mu_i}_{s_i}}}$$

Noninnovated components($\{\rho_j, k\} \neq \{s_i, \mu_i\}$)

$$\dot{\tilde{c}}^{\rho_j}_k = \tilde{f}^{\rho_j}_k (\tilde{\mathbf{c}}_{k-1}, \tilde{\mathbf{c}}_k, \tilde{c}^{\rho_j}_{k+1}, \hat{\mathbf{c}}_{k-1}, \hat{\mathbf{c}}_k, \hat{c}^{\rho_j}_{k+1}) \tag{8b}$$

where $\tilde{f}^{\mu_i}_{s_i} := \tilde{f}^{\mu_i}_{s_i}(\tilde{\mathbf{c}}_{k-1}, \tilde{\mathbf{c}}_k, \tilde{c}^{\rho_j}_{k+1}, \hat{\mathbf{c}}_{k-1}, \hat{\mathbf{c}}_k, \hat{c}^{\rho_j}_{k+1})$ and $\tilde{c}^{\mu_i}_{s_i} \approx \frac{\tilde{T}_{s_i}}{\beta_{c^{\mu_i}_{s_i}}}$.

A consequently measure of the error contribution $\tilde{y}_{s_i}$ at steady-state (i.e. when $\dot{\tilde{c}}^{\mu_i}_{s_i} = 0$) is therefore given by

$$2\xi_i \omega_i \tilde{c}^{\mu_i}_{s_i} + {\omega_i}^2 \int \tilde{c}^{\mu_i}_{s_i} \approx -\tilde{f}^{\mu_i}_{s_i} + \frac{1}{\beta_{c^{\mu_i}_{s_i}}} \left(2\xi_i \omega_i \tilde{y}_{s_i} + {\omega_i}^2 \int \tilde{y}_{s_i} \right) \tag{9}$$

According to (9), a large sensitivity ($\beta_{c_{s_i}^{\mu_i}}$) signifies small error propagation, that is small contribution of $\tilde{y}_{s_i}$ in $\tilde{c}_{s_i}^{\mu_i}$.

On the other hand, from previous binary distillation column estimation (Fernandéz (2009)) and control (Castellanos Sahagún et al. (2005)) studies, it is known that a large composition gradient (at the so-called sensitive trays) coincides with large temperature gradient, which in turn signifies the rich-in-information region for estimation and control purposes. This suggests that we look at the per-component temperature gradients for the multicomponent case, according to the formula

$$\Delta T_i = T_{i+1} - T_i \approx \sum_{j=1}^{C_M} \beta_{c_i^{\rho_j}} \Delta c_i^{\rho_j} = \sum_{j=1}^{C_M} \Delta T_{c_i^{\rho_j}} \qquad (10)$$

where $\Delta c_i^{\rho_j} = c_{i+1}^{\rho_j} - c_i^{\rho_j}$ and $\Delta T_{c_i^{\rho_j}}$ is the contribution to ΔT_i due to the j-th component. Observe that the asymptotic error characterization (9) and the temperature diagram expression (10) are related through the sensitivity terms ($\beta_{c_i^{\rho_j}}$).

According to (9) and (10), the combinaton of large sensitivity ($\beta_{c_i^{\rho_j}}$) with large concentration gradients ($\Delta c_i^{\rho_j}$) yields the largest contribution ($\Delta T_{c_i^{\rho_j}}$) to the overall temperature gradient (ΔT_i). Thus, our criteria to choose measurement structure s and innovated components μ is the following: the measurements are located at the stages with largest temperature gradients (ΔT_i), and the innovation at each measurement stage is performed on the component with largest contribution ($\Delta T_{c_i^{\rho_j}}$) to the overall temperature gradient.

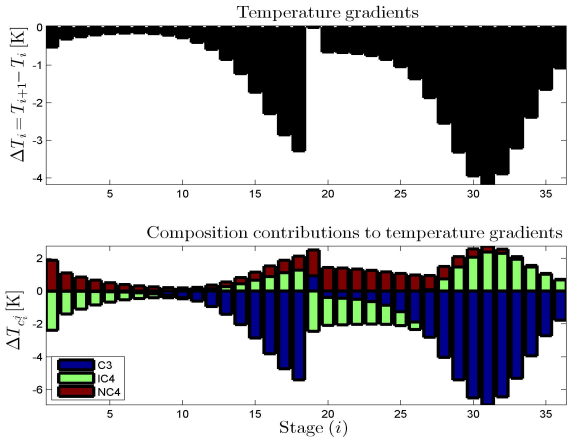

Fig. 2. SS temperature gradient and per-component contributions (10), based on the estimator model (4).

As a consequent result of these considerations, the candidate innovated states and measurement structures lead to the candidate structure set $\Sigma = \{\sigma_1, \sigma_2, \sigma_3, \sigma_4\}$ where:

$$\sigma_1 = (M, [31], \{C3\})$$
$$\sigma_2 = (M, [28, 31], \{C3, C3\})$$
$$\sigma_3 = (M, [26, 28, 31], \{C3, C3, C3\})$$
$$\sigma_4 = (M, [26, 28, 31, 33], \{C3, C3, C3, C3\})$$

These locations were chosen in the understanding that the candidate sensor locations can have variations, as long as they are in the rich-in-information region in the sense of sufficiently large per-component temperature gradient.

It must be recalled that a GE with structure σ_i has $n_M + i$ states, a number considerably smaller than the $\frac{n_M(n_M+1)}{2} + n_M$ of the equivalent EKF (Jazwinsky (1970)).

3.2 Structural results

Next, the preceding candidate structures are assessed with respect to 3-component GE functioning. For this aim, the actual 6-component system was initially set at its nominal SS and subjected to feed flow (from 88.2 to 66 $m^3\ h^{-1}$) and step-plus-sinusoidal disturbances according to the formula $c_{F,b}H(t) + c_{F,a}sin(2\pi\omega_F t)$ where $H(t)$ is a Heaviside step, $\omega_F = 10\ h^{-1}$ (chosen 4 times faster than the characteristic frequency of the measurement tray $\omega_o = 2.5\ h^{-1}$) and the $c_{F,b}$ and $c_{F,a}$ parameters are listed in Table 2. On the other hand, the 3-component GE was set with: (i) feed compositions fixed at their prescribed values c_F (listed in Table 2), (ii) sinusoidal temperature measurement noise (with amplitude of 1K and frequency $\omega_T = 20\ h^{-1}$ associated with parasitic holdup dynamics), (iii) gain frequency $\omega_i = 20\ h^{-1}$, 8 times faster than the characteristic frequency of the measurement tray ω_o, and (iv) damping factor $\xi_i = 1.5$.

Table 2. Feed composition: (i) step change for the 6-component system (2), and (ii) constant value $\hat{\mathbf{c}}_F$ for the 3-component GE (4).

	$c_{F,0}$	$c_{F,b}$	$c_{F,a}$	$\hat{\mathbf{c}}_F$
C2	0.0036	0.0064	0	
C3	0.236	0.088	0.02	0.236
IC4	0.281	−0.024	0.02	0.281
NC4	0.4746	−0.0704	−0.04	0.483
IC4	0.004	0	0	
NC5	0.0008	0	0	

In a way that is similar to the behavior assessment of controllers for distillation columns, the estimator performance is evaluated against the given estimation objective, that is the inference of the bottom C3 and distillate IC4 within the 10% relative error. For sakes of brevity, since the bottom C3 behavior is adequately inferred by the estimator model without measurement injection and no significantly changes appear when introducing component innovation, only the distillate IC4 error behavior is reported.

The GE behaviors for the model (without sensors) as well as the four candidates (1, 2, 3, and 4-measurement) structures σ_1, σ_2, σ_3, and σ_4, are illustrated in Figure 3, showing that: (i) as expected, the incorporation of measurements improves the observer behavior, and (ii) the behaviors with 3 and 4 sensors is basically the same. In what follows the behaviors will be assessed in terms of transient and asymptotic response features.

Asymptotic offset. The distillate IC4 asymptotic (relative) offset with: (i) no sensor is ≈ 408%, (ii) one sensor is larger than the prescribed tolerance (≈ 22%), (iii) two sensors is at the limit of the tolerance (≈ 9%), (iv) three sensors is about ≈ 0.3%, and (v) four sensors is about ≈ 2.5%.

Settling time. Let NST denote the natural settling time (180 min) of the estimator model. The distillate IC4 (≈

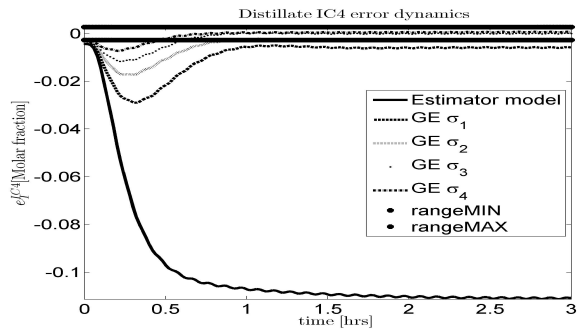

Fig. 3. Distillate IC4 composition error

98%) settling times are: (i) $\approx 0.66NST$ with one sensor, (ii) $\approx 0.5NST$ with two sensors, (iii) $\approx 0.45NST$ with three sensor, and (iv) $\approx 0.4NST$ with four sensors.

Overshoot. The distillate IC4 transient excursion (relative error) is: (i) $\approx 104\%$ with one sensor, (ii) $\approx 63\%$ with two sensors, (iii) $\approx 41\%$ with three sensors, and (iv) $\approx 25\%$ with four sensors.

According to the preceding results: (i) in the passage from zero to one measurement, the behavior undergoes a considerable improvement, (ii) the 3-component 3-sensor structure σ_3 yields the best functioning with respect to the specific (distillate IC4 and bottom C3 compositions) estimation objective, in the sense of an adequate compromise between simplicity, reconstruction speed, asymptotic offset and robustness with respect to measurement and modeling errors. Moreover, the GE with structure σ_3 needs 77 ODEs only, while the equivalent EKF would require 2849 ODEs.

In the case example, the functioning-based conclusive results are in agreement with the structural analysis-based suggestive results drawn in Section 3. In the multicomponent general case the suggestive results may undergo some refinement in the conclusive functioning assessment.

4. CONCLUSIONS

The problem of jointly designing the estimation structure and the algorithm for a multicomponent distillation column with the best estimator functioning in the light of a specific estimation objective has been addressed, with: (i) structure, meaning the number of modeled components, the innovated components, the number and locations of sensors, (ii) algorithm, meaning the dynamic data processor which performs the estimation task, and (iii) functioning meaning an adequate compromise between simplicity, reconstruction capability and robustness. The structure search problem was tractably solved with an analysis stage which yielded candidate structures followed by conclusive results based on estimator functioning. The proposed methodology was applied to a simulated industrial 6-component C3-C4 splitter where the objective is the estimation of impurity bottom C3 and distillate IC4 compositions. It was found that the best functioning was obtained with a 3-component model-based GE estimator (i) driven by three measurements located at the most sensitive region in the enriching section, and (ii) with measurement innovation in the C3 component. The resulting GE (with 77 ODEs) is considerably simpler than its EKF counterpart (with 2849 ODEs).

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