CONSTRUCTIVE ESTIMATOR DESIGN FOR BINARY DISTILLATION COLUMNS

Carlos Fernandez and Jesus Alvarez

Universidad Autónoma Metropolitana-Iztapalapa.
Departamento de Ingeniería de Procesos e Hidráulica.
Apdo. 55534, 09340 México, D.F.
MÉXICO

Abstract: The problem of jointly designing the estimation structure and algorithm for binary distillation columns is addressed within a constructive framework that combines structural and robustness concepts in the light of system characteristics. The model sensor location and number, the innovated-noninnovated state partition, and the model dimension are regarded as structural design degrees of freedom. The geometric and extended Kalman filter estimators are regards as algorithms to perform the data assimilation task. The high-order Lie derivation applicability obstacle of the geometric estimation technique is removed, and the equivalence between geometric and extended Kalman filter is established. The methodological findings and the estimator functioning results are illustrated and tested with experimental data.

Keywords: nonlinear estimator, geometric estimation, binary distillation column, detectability measures and structures.

1. INTRODUCTION

The study of the distillation column estimation problem is motivated by the need of improved monitoring and control schemes. The idea is to infer the concentration profile on the basis of a model with temperature measurements. The subject has been extensively studied, the related state of the art can be seen elswhere (Joseph and Brosilow, 1978; Lang and Gilles, 1990; Baratti et al., 1995; Baratti et al., 1998; Oisiovici et al, 2000; Castellanos et al, 2005, Tronci et al, 2005), and here it suffices to mention that: (i) distillation column have large state-to-measurement ratios, meaning high observability indices, (ii) the best estimator behaviors have been attained with the extended Kalman filter (EKF) technique, including ternary systems, (iii) the Luenberger and geometric estimation approaches become inapplicable due to the intractability of high-order Lie derivative calculations, (iv) the estimator design involves both structure and algorithm decisions, (v) some model reduction techniques have been employed (Mejdell and Skogestad, 1991), and (vi) in spite of some efforts via observability measures, the selection of the number of sensors and their locations is still an open subject of research. These considerations motivate the study of joint structure-algorithm estimation problem. According to the constructive approach, an optimality-based robust control design, over a set of candidate structures, can be tractably pursued by combining geometric and error propagation analysis tools in the light of specific systems characteristics (Sepulchre et al, 1997; Krstić et al, 1990). These ideas have been developed mostly in the context of control problems for mechanical and electrical systems, and have been recently applied to distillation column (Castellanos et al, 2005; Castellanos and Alvarez 2006, Castellanos et al, 2006) and polymer reactor (Alvarez et al, 2004; Gonzalez and Alvarez, 2005; Alvarez and Gonzalez 2007) control schemes with interlaced estimator-control designs made of PI and inventory control components.

Along this constructive line of thought, the adjustable-structure geometric estimation technique has been developed in the context of systems with low state-to-measurement ratios like chemical reactors (Alvarez 2004; Lopez and Alvarez, 2004). This technique (i) does not need to on-line solve Riccati equations, but cannot be applied to systems with large state-to-measurement ratios with high observability indices, like distillation columns, because the computation of high-order Lie derivatives becomes an intractable task (Tronci et al, 2005; Röbenack, 2005; Venkateswarlu and Kumar, 2006), and (ii) lacks a formal connection with the EKF that is the one that better handles the distillation column estimation problem. Recently (Fernandez, 2007; Alvarez and Fernandez, 2007), the high estimation order applicability obstacle of the geometric estimator has been removed, and the geometric estimator (GE) has been formally connected with the EKF. These considerations are points of departure for the present study.

In this paper, the problem of jointly designing the estimation structure and algorithm for binary distillation columns is addressed within a constructive framework that combines structural and robustness concepts in the light of system characteristics. The model sensor location and number, the innovated-noninnovated state partition, and the model dimension are regarded as structural design degrees of freedom. The geometric and EKF estimators are regarded as candidate algorithms to perform the data assimilation task. The removal the high-order Lie derivation applicability obstacle of the geometric estimation technique, and its equivalence between geometric and EKF are verified. The methodological findings and the estimator functioning results are illustrated and tested with experimental data.

2. ESTIMATION PROBLEM

2.1 Estimation problem

Consider the N-tray binary distillation column, where a binary mixture, with molar flow F and light-component mole fraction composition c_F, is fed at tray n_F, yielding effluent flow B (or D) with composition (c_B) (or c_D). V is the internal vapor flow (proportional to the heat rate exchanged in the boiler), R is the reflux flow rate, and T_i is the temperature measurement at the i-th stage. Without restricting the approach, a total condenser is considered. Under standard assumptions (constant pressure, equilibrium in all stages, level control in the reboiler, constant molar flows, and liquid flow dynamics in quasi steady-state), the *column model* is given by (Luyben, 1990)

$$\dot{c}_1 = \{(R+F)(c_2 - c_1) - V[\varepsilon(c_2) - c_1]\}/M_1 := f_1, \quad c_B = c_1$$

$$\dot{c}_i = \{L(c_{i+1} - c_i) - V[\varepsilon(c_i) - \varepsilon(c_{i-1})] + \delta_{i,n_F}F(c_F - c_{n_F})\}/\eta^{-1}(L)$$

$$:= f_i,\ 2 \le i \le n; \qquad T_j = \beta(c_{sj}), \qquad 1 \le j \le m$$

$$\dot{c}_n = \{R\varepsilon(c_n) - V[\varepsilon(c_n) - \varepsilon(c_{n-1})]\}/\eta^{-1}(L) := f_n, \quad c_D = \varepsilon(c_n)$$

$$L = R + F\ \forall\, i \in [2, n_F], \qquad L = R\ \forall\, i \in [\,n_F+1, n]$$

where ε, β, and η denote the liquid-vapor, bubble point, and (Francis weir) hydraulics functions, respectively. In vector notation, this column model is written as follows:

$$\dot{x} = f(x, u),\ y_m = h(x);\ x = (c_1,\ldots,c_n)',\ u_p = (d',u')' \quad (1)$$

$$d = (F, c_e)', \qquad u = (R, V)', \qquad h_i = \beta(c_{sj}), \quad 1 \le j \le m$$

The *estimation problem* consists in inferring the composition profile on the basis of a sensor set with number and locations to be determined. We are interested in: (i) verifying the functioning of the above mentioned redesigned GE, without needing Lie derivatives, and its connection with the EKF estimation, (ii) the comparison of the geometric approach-based detectability measures with previous ones, and (iii) the extent to which the structure and algorithm estimation choices affect the estimator behavior.

2.2 Experimental run

Apparatus. A laboratory glass column (model IC18-DV/92, Didacta-Italy) was employed to generate the experimental data, with: 11 oldershaw-type trays, evaporator, total atmospheric condenser, thermo-siphon type boiler, and electric heating. The feed and bottoms flows were set with digital peristaltic pumps, and the reflux flow was regulated with a solenoid valve. A binary methanol-water mixture was separated, temperature was on-line monitored in six stages (trays 1, 3, 5, 7, 9 and 11, evaporator, and condenser), and composition were sampled (each 5 min) at the same stages, and off-line determined via densitometry. The corresponding experimental data are shown in Figures 1, 4 and 5.

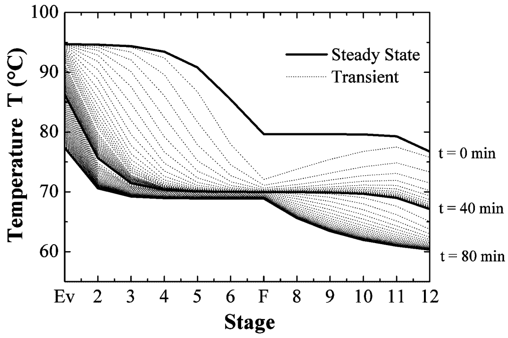

Fig. 1. Experimental temperature profiles evolution

Test motion. To subject the estimators to a severe test, with state evolutions over an ample region of the column state-space, a drastic transient column response was set as follows. The (saturated) feed was set at F = 40 ml/min, with light component composition c_e = 0.2 and temperature 57°C. Initially the column was at a steady-state with low reflux ratio (R/D = 0.2) and poor separation ($c_B \approx 0.0$, $c_D \approx 0.57$). Then, at time t = 0, a step increase (up to c_e = 0.4) of feed composition was introduced, yielding a response that settled in about 40 min with intermediate separation ($c_B \approx 0.01$, $c_D \approx 0.79$). Finally, at t = 40 min, a reflux step increase (up to R/D = 1.5) was introduced, yielding a response that settled in about 40 min., with high separation ($c_B \approx 0.15$, $c_D \approx 0.98$). The corresponding temperature profile evolution is presented in Figure 1.

3. GEOMETRIC AND EKF ESTIMATION

In this section the redesigned GE method is applied to our distillation column, with one difference: the thermodynamic and staged characteristics of the distillation process are exploited. Emphasis is placed on the verification of the feasibility of removing of the high-order Lie derivation obstacle and shows the GE-EKF connection.

3.1. Geometric Estimator

Assuming the column model (1) motion x(t) is *detectable with structure* σ (*σ-detectable*), the corresponding (redesigned) geometric estimator is given by:

$$\dot{\hat{x}}_\iota = f_\iota(\hat{x}, u) + O^{-1}(\hat{x}, u)\{\Pi\hat{\iota} + K_y[y(t) - h(\hat{x})]\} \quad (2a)$$

$$\dot{\hat{\iota}} = K_\iota[y - h(\hat{x})], \qquad \dot{\hat{x}}_v = f_v(\hat{x}, u) \quad (2b)$$

where (I_x is a column-permuted identity matrix)

$$(f_\iota', f_v')' = I_x f, \qquad \dim(\hat{x}_\iota, \hat{x}_v, \hat{\iota}) = (\kappa_\iota, n - \kappa_\iota, m)$$
$$\kappa_\iota = \kappa_1 + \ldots + \kappa_m \le n, \qquad \kappa_i > 1$$
$$O(x, u) = [O_1'(x, u) \ldots, O_m'(x, u)]' \quad (3)$$
$$O_i'(x, u) = [c_i(x, u), \ldots, c_i(x, u)A^{\kappa_i - 1}(x, u)]$$
$$A(x, u) = \partial_x f(x, u), \qquad c_i(x) = \partial_x h_i(x)$$

$\hat{x}_\iota$ (or $\hat{x}_v$) is the *innovated* (or *noninnovated*) state and $\hat{\iota}$ is an augmented state that eliminates the output mismatch, O is the *estimation matrix*, and Π, Γ_u and Δ_u are zero/one-entry matrices with structure determined by κ (Lopez and Alvarez, 2004). The matrix gain pair (K_y, K_ι) (4), and the related output quasi linear noninteractive pole assignable (qLNPA) estimation error dynamics (5) are given by

$$K_y = \mathrm{bd}[k_1^y, \ldots, k_m^y], \qquad k_i^y = (a_1^i\omega_i, \ldots, a_{\kappa m}^i\omega_i^{\kappa i})' \quad (4a)$$
$$K_i = (\omega_1^{\kappa 1+1}, \ldots, \omega_m^{\kappa m+1})', \quad c_i = (a_{\kappa m+1}^i, \ldots, a_1^i) \quad (4b)$$
$$\mathcal{L}_{yi}\tilde{y}_i := \tilde{y}_i^{(\kappa_i+1)} + (a_1^i\omega_i)\tilde{y}_i^{(\kappa_i)} + \ldots + (a_{\kappa_i+1}^i\omega_1^{(\kappa_i+1)})\tilde{y}_i \approx 0 \quad (5)$$
$$\tilde{y}_i = \hat{y}_i - y_i, \; 1 \le i \le m$$

where c_i is the coefficient set of a monic, unit frequency, normalized (κ_i+1)-order polynomial set by a prescribed pole pattern, and ω_i is the characteristic frequency, or equivalently, the speed parameter of the of the i-th output error dynamics. The *estimation structure* σ is given by

$$\sigma = (\kappa, x_\iota\text{-}x_v): \kappa = (\kappa_1, \ldots, \kappa_m)', \; (x_\iota', x_v')' = I_x x \quad (6)$$

where κ is the estimation order vector, x_ι-x_v is the innovated-noninnovated state partition, and κ_ι is the *estimation order* associated with the i-th output.

Basically, σ-detectability is a robustness-oriented coordinate-dependent version of the coordinate-free definition of k-differential nominal detectability (Sontag, 2000). In our distillation column, structure means: the sensor number and locations, the innovated-noninnovated state partition, and the innovated states per measurement. When the n (or less than n) model states are innovated, the structure is said to have *complete (or partial) innovation* with $\kappa = n$ (or $\kappa < n$)

3.2. Conventional EKF (CEKF)

Motivated by the GE form (2), let consider the stochastic version

$$\dot{x} = f(x, u) + B(x, u)w(t), \; \hat{x}(0) = \hat{x}_o, \; y = h(x) + v(t) \quad (7)$$

of the column model (Eq. 1), where w (or v) is a zero-mean Gaussian white noise with intensity matrix R (or Q). The corresponding *EKF* is given by:

$$\dot{\hat{x}} = f(\hat{x}, \hat{u}) + S_x C'(\hat{x})R^{-1}[y - h(\hat{x})], \; \hat{x}(0) = \hat{x}_o \quad (8a)$$

$$\dot{S}_\iota = Q - S_\iota[h_x'(\hat{x})R^{-1}h_x(\hat{x})]S_\iota, \qquad S_\iota(0) = S_{\iota o} \quad (8b)$$

$$\dot{S}_{\iota x} = S_{\iota x}F(\hat{x}, \hat{\iota}, u) + S_{\iota x}H(\hat{x}, u) \quad (8c)$$
$$- S_{\iota x}[C'(\hat{x})R^{-1}C(\hat{x})]S_x, \qquad S_{\iota x}(0) = S_{\iota xo}$$

$$\dot{S}_x = F(\hat{x}, \hat{\iota}, u)S_x + S_x F'(\hat{x}, \hat{\iota}, u) \quad (8d)$$
$$+ B(\hat{x}, \hat{u})S_\iota B'(\hat{x}, \hat{u}) + H(\hat{x}, u)S_{\iota x} + S_{\iota x}'H'(\hat{x}, u)$$
$$- S_x[C'(\hat{x})R^{-1}C(\hat{x})]S_x, \qquad S_x(0) = S_{xo}$$

where $F(x, \iota, u) = \partial_x[f(x, u) + B(x, u)\iota]$

$$H(x, u) = \partial_\iota[B(x, u)\iota], \qquad \begin{bmatrix} S_\iota & S_{\iota x} \\ S_{\iota x}' & S_{xo} \end{bmatrix} = S$$

ι is a colored noise, and $x_{\iota o}$ (or ι_o) is a random vector with mean $\hat{x}_{\iota o}$(or $\hat{\iota}_o$) and error covariance matrix S_{xo} (or $S_{\iota o}$). In most distillation column studies (Barati et al, 1995, Oisiovici et al, 2000): (i) (B, ι) = (I, w) (ι is a white noise, and the i-th error w_i enters the i-th state dynamics), (ii) the matrix R_{mxm} (or Q_{nxn}) is set in diagonal (or block diagonal) form with a reduced number of adjustable entries, and (iii) $S_o = 0$ because the EKF is quite robust with respect to the choice of S_o. In most cases, the adjustable entries of (R, Q) are tuned by trial-and-error, and occasionally with off-line optimization procedures.

3.3. Geometric-EKF equivalence

The GE and EKF designs coincide if: (i) The gain pair of the GE (Eq. 4) is set with Butterworth pole patterns, (ii) the noninnovated dynamics are in slow-varying regime with respect to the innovated dynamics, and (iii) The EKF (Eq. 8) is set with (Σ is the solution of Eq. 9c)

$$R = \mathrm{dg}(r_1, \ldots, r_m), Q = \mathrm{dg}(q_1, \ldots, q_m), q_i = r_i(\omega_i)^{2(\kappa i + 1)} \quad (9a)$$
$$B(x, u) = O^{-1}(x, u)\Pi, S_o = O^{-1}(\hat{x}_o, \hat{u}_o)\Sigma_z O^{-1\prime}(\hat{x}_o, \hat{u}_o) \quad (9b)$$
$$0 = \Gamma\Sigma + \Sigma\Gamma' + \Pi Q\Pi' - \Sigma\Delta' R^{-1}\Delta\Sigma, \Sigma = \begin{bmatrix} \Sigma_\iota & \Sigma_{\iota z} \\ S_{\iota z}' & \Sigma_z \end{bmatrix} \quad (9c)$$
$$\dim \Sigma = (\kappa_\iota + 1, \kappa_\iota + 1), \qquad m \le \kappa_\iota \le n$$

$\{\Gamma, \Delta, \Pi\}$ is a set of zero/one-entry matrices. From this equivalence, the *stochastic geometric estimator* follows:

$$\dot{\hat{x}}_\iota = f_\iota(\hat{x}, u) + O^{-1}(\hat{x}, u)\{\Pi\hat{\iota} + K_y[y(t) - h(\hat{x})]\} \quad (10a)$$

$$\dot{\hat{\iota}} = K_\iota[y - h(\hat{x})], \qquad \dot{\hat{x}}_v = f_v(\hat{x}, u) \quad (10b\text{-}c)$$
$$S_x = O^{-1}(\hat{x}, \hat{u})\Sigma_z(\omega_e)\, O^{-1\prime}(\hat{x}, \hat{u}), \quad \tilde{x} = \hat{x} - x \quad (10d\text{-}e)$$

where the dynamic-decoupled component (10a) yields the mean state estimate ($\hat{x}$), and the static component (10d) yields the estimate uncertainty assessment (S_x).

4. STRUCTURE DESIGN

Following the constructive approach, the structure choice, over a large number of candidates, must be done by exploiting the staged nature of the column as well as its material balance and thermodynamic features in the light of the adjustable-structure feature of the geometric estimation approach and of its detectability measures (Lopez and Alvarez, 2004).

4.1 Estimation structures

The set of *admissible structures* σ is denoted by S_A, and the subsets of *detectable* (or *passive*) *structures* is denoted by S_D (or S_P) (Lopez and Alvarez, 2004):

$$S_A = \{\sigma |\, x(t) \text{ is } \kappa\text{-detectable}\}$$
$$S_D = \{\sigma \in S_\sigma \,|\, \kappa_d = \max_{S_A} \kappa_\iota\}; \; S_P = \{\sigma \in S_\sigma \,|\, \kappa_i = 1\}$$

The detectable (or passive) structure signifies maximum (or minimum) innovated state dimension κ_d (or m), largest (or smallest) state reconstruction rate, and smallest (largest) robustness. The structure choice amounts to a suitable compromise between state reconstruction speed and robustness. In our 12-state distillation column example with up to 12 sensors (i.e., n= 12, $1 \leq m \leq 12$, and $1 \leq \kappa_\iota \leq 12$) we have: card S_A = 527,345 admissible structures with card S_D (or S_P) = 4,095 observable (or passive) structures.

4.2 Structural assessment

Next the structure selection is performed on the basis of: (i) the staged nature of the process, in the sense of the profile monotonicity (Sontag, 2000), or equivalently, the order feature of the compositions and their unidirectional change with the exogenous inputs, and (ii) the geometric approach-based detectability measures (Lopez and Alvarez, 2004):

$$\mu_c = \mathrm{cn}[O(x, u, \kappa)], \qquad \mu_s = \sigma_{\min}^{-1}[O(x, u, \kappa)] \quad \text{(11a-b)}$$

$$\mu_c^v = \mathrm{cn}[J(x, u, \kappa)], \qquad J(x, u, \kappa) = (F + F')/2 \quad \text{(11c)}$$

$$F(x, u, \kappa) = (\partial_{x_v} f_v + \partial_{x_\iota} f_v)(\partial_{x_v} x_\iota)(x, u, \kappa)$$

$$\lambda_v = \min\,[-\mathrm{Re}(\lambda_1),\ldots,-\mathrm{Re}(\lambda_{n-\kappa})], \qquad F x_i = \lambda_i x_i \quad \text{(11d)}$$

where cn (or $\sigma_{\min}$) $(\cdot)$ is the condition number (or minimum singular value) of $(\cdot)$, μ_c (or μ_s) measures the ill-conditioning (or singularity) of the estimation matrix O, and μ_c^v (or λ_v) measures the ill-conditioning (or stability-speed) of the noninnovated dynamics. As the innovated state dimension (κ) is increased: (i) the ill-conditioning (μ_c) and singularity (μ_s) of O grow, or equivalently, the model error propagation by measurement injection grows, and (ii) the ill-conditioning (or stability margin) of the noninnovated dynamics decreases (or increases). These error propagation features must be considered in the light of the before stated nominal features: as the estimation (κ) order grows, the innovated state dimension grows, signifying a fastest reconstruction speed.

For comparison purposes, let us regard the detectability measure pair (μ_c, μ_s) (11) on the basis of the Grammian matrix (Hahn and Edgar, 2002) W_o which is given by the solution of the matrix equation:

$$W(x, u, \kappa) \ni A'(x, u, \kappa)\, W_o + W_o\, A(x, u, \kappa) - C'(x, u, \kappa)C(x, u, \kappa) = 0 \quad (12)$$

It has been claimed that, for measurement choice purposes, the observability and Grammian matrices yield the same results (Johnson, 1969).

Single-sensor analysis. The application of the preceding detectability measures (11) to our case example yielded that: (i) the binary column is (nominally) completely observable with at least one sensor located at any stage, and this agrees with previous reports drawn from linear analyses (Joseph and Brosilow, 1978), (ii) the measures (μ_c^v and λ_v) associated with the noninnovated dynamics do not change significantly with structure, (iii) the singularity measure μ_s (11b) (that, in an IS stability framework, signifies the asymptotic estimation error gain) reflects the estimator behavior-structure dependency in a better way better than the ill-conditioning measure μ_c (11a), and (iv) the singularity measures (11b) on the basis of the

a)

b)

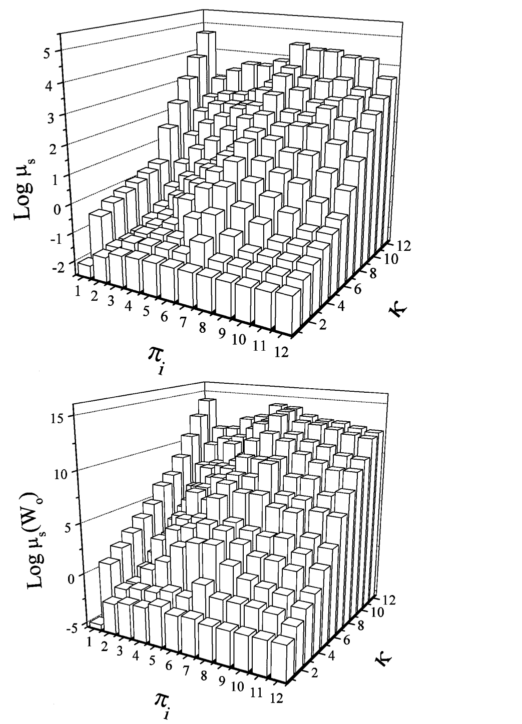

Fig. 2. Single-sensor singularity measure (μ_2) dependency on sensor location (π_i) and estimation order (κ), at t = 40 min, using estimation (a) and Grammian (b) matrices.

observability (3) and Grammian matrices (12) yield the same structural assessments.

In Figure 2 are plotted the dependencies of the singularity (μ_s) measure on the single-sensor location and the estimation order (i.e., dim x_ι), showing that: (i) as expected, low innovation dimensions yield the smallest error propagation by measurement injection, (ii) for complete innovation structures order (with κ =12) the sensors in stages 2 (1st tray) and 12 (11th tray) yield the smallest error propagation, or equivalently, the maximum robustness, and these locations coincide with the largest stage-to-stage temperature and concentration changes, and (iii) for partial innovation structures (i.e., with $1 < \kappa < 12$) a single sensor should be located either in the stripping (or enriching) section location set {1, 2, 3, 4} (or {9, 10, 11, 12}. Moreover, the comparison of Figures 2a and 2b verifies the above stated claim drawn from theoretical arguments: that the singularity measures with estimation and Grammian matrix yield the same structural result.

Multiple-sensor structure. Due to the column staged nature and monotonicity property (Sontag, 2000), from the preceding single-sensor structural analysis in conjunction with Figure 2a the multiple-measurement structural suggestions follows: (i) two measurements should be used, one per section, (ii) in each section, the sensor must be located in the (above delimited) most sensitive region, and (iii) no more that three innovated states per measurement are needed to perform the full profile estimation task. These suggestions were ratified on the basis of the results presented in Figure 3, that presents the changes of the ill-conditioning and singularity estimation matrix measures with the number of optimally located sensors, showing that: (i) there is a

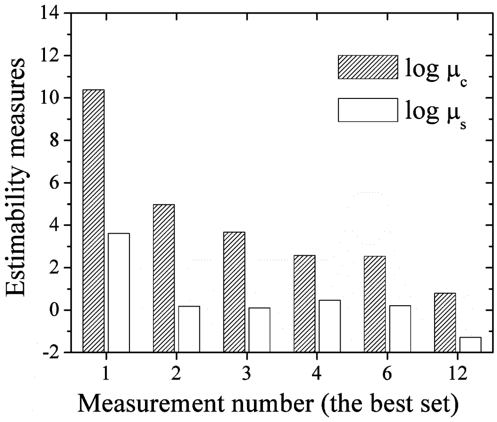

Fig. 3. Ill-conditioning and singularity measure dependencies on the number of optimally placed sensors.

significant improvement from one to two sensors, and (ii) the incorporation of more sensors does not yield an appreciable improvement.

5. ESTIMATOR BEHAVIOR

In this section the functioning of the redesigned GE (without Lie derivation) is tested, the GE-EKF equivalence will be assessed, and the structural findings will be tested with geometric and EKF algorithms (dynamic data processors).

5.1 Tuning

Following the structural assessment conclusions, the estimation scheme was set with two sensors located at stages 2 and 12. *The GE* was tuned with complex Butterworth pole placement (i.e., damping factor $\zeta = 2^{1/2}$), and frequency pair $(\omega_s, \omega_e) \approx (2/5, 2/10)$ found by starting at $\omega_s = \omega_e := \omega \approx 10\lambda_c$ (the dominant column frequency), increasing until an ultimate value $\omega^* \approx \lambda_h$ (hydraulics frequency) with oscillatory behavior, followed by backoff $\omega^*/2$, and final refinement. *The CEKF* (8) was set with the block diagonal structure (Baratti et al, 1995):

$$B(x, u) = I_{12x12}, \qquad Q = bd(q_s I_{6x6}, q_e I_{6x6}) \qquad (13)$$
$$q_s = r(\omega_s)^{14}, \qquad q_e = r(\omega_e)^{14}, \qquad r = 0.5$$

with one difference: here, (q_s, q_e) was not set by trial-and-error, but with the value of (ω_s, ω_e) of the GE tuning in conjunction with the GE-EKF equivalence formula (9a), verifying that not appreciable improvement was obtained by further adjusting (q_s, q_e). The value of (ω_s, ω_e) was kept fixed over different estimation structures and algorithms.

5.1 SGE, CEKF and GEKF estimation with complete innovation.

In a comparison between the GE (2, 10) and CEKF (8, 13) approaches with two optimally located sensors, the complete-innovation structure represents the most unfavorable situation for the GE. This is so because, while the CEKF can be implemented and tuned for an adequate functioning, the original Lie derivative-based GE could only be implemented up to three innovated states per sensor, meaning three Lie derivations less than the ones required by the complete innovation structure. The *SGE (10)* and *GEKF (9)* were implemented with the structure

$$\sigma = (\kappa, x_\iota = x), \quad x = (c_1, \ldots, c_{12})', \qquad \kappa_s = \kappa_e = 6$$

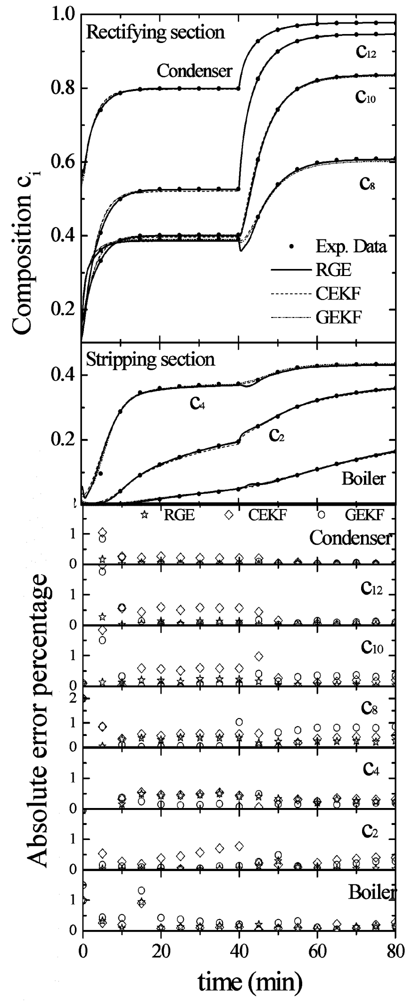

Fig. 4. *SGE, CEKF and GEKF estimation with complete innovation.*

The behaviors of the GE (13 ODEs), GEKF (104 ODEs) and CEKF (with 104 ODEs) are presented in Figure 4, showing that: (i) the redesigned GE effectively removes the Lie derivation applicability obstacle of the original geometric estimator (Alvarez, 2000), (ii) the GE and GEKF yield the same behavior, verifying the GE-EKF equivalence, and (iii) the GE estimator without Riccati equations (REs) yields the same estimates than the CEKF with REs. As it can be seen in Figure 5, the CEKF and SGE yield the same uncertainty assessment, which closely resemble the actual ones drawn from the off-line concentration measurements.

5.2 SGE and GEKF estimation with partial innovation.

Following the structure assessment results, let us consider the partial-innovation estimation structure:

$$\sigma = (\kappa, x_\iota - x_v), \; x_\iota = (c_1, c_2, c_3, c_{10}, c_{11}, c_{12})'$$
$$x_v = (c_4, c_5, c_6, c_7, c_8, c_9)'$$

meaning that only six states undergo direct measurement injection. The resulting behaviors with GE (14 ODEs) and GEKF (34 ODEs) is presented in Figure 5, showing that: (i) the two estimators yield the same behavior, and (ii) such behavior is not significant different from the ones drawn with complete innovation (Figure 4).

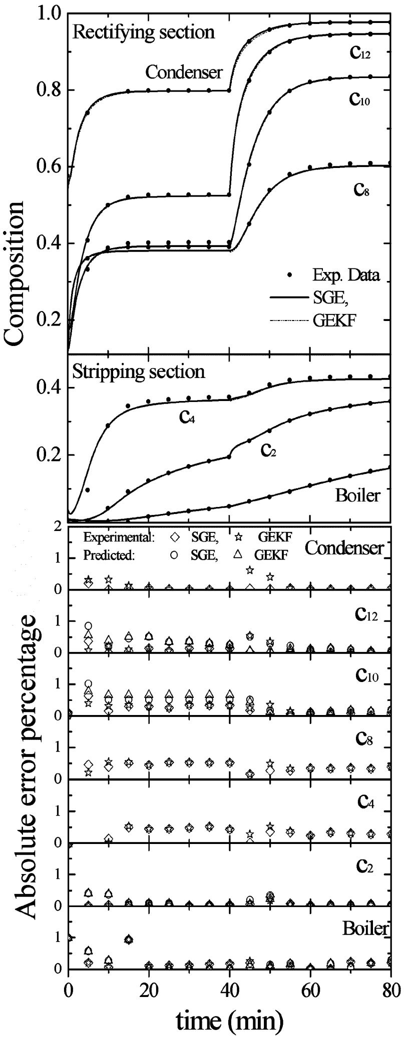

Fig. 5. *SGE and GEKF estimation with partial innovation*

6. CONCLUSIONS

The structure-algorithm estimation problem for binary distillation columns has been addressed via a constructive approach. The estimation structure was *a priori* assessed according to detectability measures and staged process features in the light of estimator functioning. It was verified that the redesigned GE: (i) eliminates the cumbersome or intractable Lie derivations of its original counterpart, (ii) is equivalent to an EKF with a special model injection uncertainty model, (iii) circumvents the need of on-line integrating Riccati. The GE-EKF equivalence enabled the uncertainty assessment capability of the GE.

It was found that (i) the structural decisions plays a key role in the estimator behaviour, regardless of the particular estimation algorithm employed (i) the best estimator functioning is obtained by injecting the temperature measurement-based information over a few column states and this is in agreement with the industrial practice on sensor location distillation control criteria. The methodological findings and the estimator functioning results were illustrated and tested with experimental data.

REFERENCES

Alvarez, J. (2000). "Nonlinear state estimation with robust convergence", *J. Process Control,* **10**: 59-71

Alvarez J. and Fernandez C. (2007). "Constructive estimation of nonlinear process: application to an experimental distillation column". paper in preparation.

Alvarez, J. and González, P. (2007) “Constructive control of continuous polymer reactors” *J. Process. Control.*, **17**: 463-476 .

Alvarez. J., Zaldo, F. and Oaxaca, G. (2004). “Towards a Joint Process and Control Design Approach for Batch Processes: Application to a Polymer Reactor” Cap D6, pp 604-634 J. In the book “Integration of process and Control Design”, Michael Georgadis y Stavros Panos (Editors), Elsevier, Amsterdam.

Baratti, R., Bertucco, A., Da Rold, A. and Morbidelli, M. (1995). "Development of a Composition Estimator for Binary Distillation Columns: Application to a Pilot Plant", *Chem. Eng. Sci.*, **50**: 1541-1550

Baratti, R., Bertucco, A., Da Rold, A. and Morbidelli, M. (1998). "A composition estimator for multicomponent distillation columns-development and experimental test on ternary mixtures", *Chem. Eng. Sci.*, **53**: 3601-3612

Castellanos Sahagún, E., Alvarez-Ramírez, J., Alvarez, J. (2005). "Two-Point Control Structure and Algorithm Design for Binary Distillation Columns", *Ind. Eng. Chem. Res*, 44: 142-152

Castellanos Sahagun, E., Alvarez, J. (2006). “Synthesis of two-point linear controllers for binary distillation columns” Chem. Eng. Commun., **193**: 206-232

Castellanos Sahagun, E., Alvarez, J. and Alvarez-Ramírez, J., (2006). “Two-point composition-temperature control of binary distillation columns” *Ind. Eng. Chem. Res*, in press.

Fernandez, C. (2007). Estimation of binary ditillation columns, PhD thesis (in Spanish), Universidad Autónoma Metropoolitana, México

Gonzalez, P. and Alvarez, J. (2005). "Combined proportional/integral-inventory control of solution homopolymerization reactors." *Ind. Eng. Chem. Res*. **44**: 7147-7163.

Hahn, J. and Edgar, T. F. (2002). "An improved method for nonlinear model reduction using balancing of empirical gramians", *Comput. Chem. Eng*. **26**: 1379-1397

Johnson, C. D. (1969). "Optimization of a Certain Quality of Complete Controllability and Observability for Linear Dynamical Systems". *Transactions of the ASME*, 228-238.

Joseph, B. and Brosilow, C. B. (1978). "Inferential Control of Processes: Part I. Steady Analysis and Design", *AIChE J.*, **24**: 485-492

Krstić, M., Kanellakopoulos, I. and P. Kokotović (1995). Nonlinear and adaptive control design, Wiley Interscience.

Lang, L. and Gilles, E. D. (1990). "Nonlinear Observers for Distillation Columns", *Comput. Chem. Eng*. **14**: 1297-1301

López, T. and Alvarez, J. (2004). "On the effect of the estimation structure in the functioning of a nonlinear copolymer reactor estimator". *J. Process Control*, **14**: 99-109

Luyben, W. L. (1990). Process modelling simulation and control for chemical engineers. 2nd Ed. McGraw-Hill, New York.

Mejdell, T. and Skogestad, S. (1991). "Estimation of Distillation Compositions from Multiple Temperature Measurements Using Partial-Least-Squares Regression", *Ind. Eng. Chem. Res*. **30**: 2543-2555

Oisiovici, R. M. and Cruz, S. L. (2000). "State estimation of batch distillation columns using an extended Kalman filter", Chem. Eng. Sci., **55**: 4667-4680

Röbenack, K. (2005) "Computation of High-Gain Observers for Nonlinear Systems Using Automatic Differentiation", Transactions of the ASME, **127:** 160-162.

Sepulchre, R., Janković, M., Kokotović, P. R. (1997) Constructive Nonlinear Control, Communications and Control Engineering Series, Springer - Verlag, London

Sontag. E. D. (2000) The ISS philosophy as a unifying framework for stability-like behavior, in: A. Isidori, F. Lamnabhi-Lagarrigue, W. Respondek (Eds.), Nonlinear Control in the Year 2000, Lecture Notes in Control and Information Sciences, vol. 2, Springer-Verlag, Berlin, pp. 443–468.

Tronci, S., Bezzo, F., Barolo, M. and Baratti, R. (2005)."Geometric observer for a distillation column: development and experimental testing." *Ind. Eng. Chem. Res.*, **44**: 9884-9893

Venkateswarlu, C. and Jeevan Kumar, B. (2006). "Composition estimation of multicomponent reactive batch distillation with optimal sensor configuration." *Chem. Eng. Sci.,* **61**: 5260-5274