Geometric Estimation of Binary Distillation Columns

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Abstract: The problem of designing the estimation structure to perform a specific (entire profile, single/two-effluent, and so son) concentration estimation task in a binary distillation column with two temperature measurements is addressed within a geometric estimation (GE) framework. The structure design involves the choices of: (i) the measurement locations, (i) the complete or truncated estimation model, and (iii) the innovated-noninnovated state partition of the model. First, a structural analysis is performed on the basis of detectability measures in the light of the column characteristics, yielding candidate structures for a specific estimation task. Then, the behavior of the structures is assessed with estimator functioning and dimension considerations, yielding conclusive structural results. The proposed methodology is applied to a representative case example with experimental data.

Keywords: Nonlinear estimator, geometric estimator, nonlinear system realization, distillation column estimation.

1. INTRODUCTION

The study of the concentration estimation problem for distillation columns is motivated by the development of advanced monitoring and control schemes. The estimator design involves decisions on: (i) the structure (sensor number and locations), and (ii) the kind of (EKF, Luenberger, Geometric, etc) algorithm. In the distillation column estimation field: (i) the EKF has been, by far, the most widely employed and accepted algorithm, (ii) the sensor structure has been decided with heuristics (Oisiovici and Cruz, 2000) or observability measures (van der Berg et al. 2000; Singh and Hahn, 2005), (ii) only in a few studies (Alonso et al, 2004; Bian and Henson 2006; Venkateswarlu and Kumar, 2006; Kadu et al, 2008) the measure-based sensor location results have been tested with estimator functioning and is not clear to what extent the results depend on tuning. In principle, the resolution of this drawback requires a unified framework to address the algorithm, sensor location, and tuning aspects.

Recently (Alvarez and Fernandez, 2009), the general-purpose nonlinear geometric estimator (GE) (Alvarez and Lopez, 1999; Alvarez 2000) has been redesigned with: (i) an implementation in terms of model Jacobian matrices (and not of the cumbersome or intractable Lie derivation-based gain of the nonlinear Luenberger observer), (ii) the structure (sensors, complete/truncated model, innovation scheme) as a key design degree of freedom, and (iii) a simple tuning procedure based on a robust convergence criterion, regardless of the structure, and (iv) testing with an experimental binary distillation column. This adjustable-structure GE methodology and the associated nonlinear detectability measures (Lopez and Alvarez, 2004) constitute the methodological points of departure for the present study.

In this work, the problem of designing the best estimation structure (in terms of reconstruction speed, robustness, and algorithm simplicity) to perform a specific (entire profile or two-effluent) concentration estimation task in a binary distillation column with two temperature measurements is addressed, with structure meaning the choices of: (i) the *measurement locations*, (i) the (complete or truncated) *estimation model*, and (iii) the innovated-noninnovated model *state partition*. The proposed methodology is applied to a representative case example with experimental data.

2. ESTIMATION PROBLEM

2.1 Column system and model

Consider an N-stage binary distillation column, with molar feed flow F in tray n_f at (light-component) mole fraction c_F, and bottoms (or distillate) flow B (or D) at composition c_B (or c_D), and a total condenser. Under standard (constant pressure, stage equilibrium, fast holdup dynamics with perfect mixing, evaporator level control, constant molar flow, saturated feed, and adiabatic system) assumptions the *N-composition column model* is given by (Luyben, 1990)

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

$$\dot{c}_i = \{(R + F)(c_{i+1} - c_i) - V[\varepsilon(c_i) - \varepsilon(c_{i-1})]\}/\eta^{-1}(R + F) := f_i,$$
$$1 \le i \le n_f - 1, \qquad \eta(M) = a_\eta(M - M_o)^{b_\eta}$$

$$\dot{c}_{nf} = \{(R + F)(c_{nf+1} - c_{nf}) - V[\varepsilon(c_{nf}) - \varepsilon(c_{nf-1})] + F(c_F - c_{nf})\}/\eta^{-1}(R + F) := f_{nf}$$

$$\dot{c}_i = \{R(c_{i+1} - c_i) - V[\varepsilon(c_i) - \varepsilon(c_{i-1})]\}/\eta^{-1}(R) := f_i, \quad n_f + 1 \le i \le n-1$$

$$\dot{c}_N = \{R[\varepsilon(c_N) - c_N] - V[\varepsilon(c_N) - \varepsilon(c_{N-1})]\}/\eta^{-1}(R) := f_N, \; c_D = \varepsilon(c_N)$$
$$y_1 = T_1 = \beta(c_{l_1}), \qquad y_2 = T_2 = \beta(c_{l_2})$$

c_i is the i-th stage mol fraction of light component, V (or R) is the vapor (or reflux) flow, M_i is the i-th stage molar holdup, and T_i is the temperature measurement at the l_l-th stage, ε, β, and η are the liquid-vapor, bubble point, and (Francis weir equation) hydraulics functions, respectively. Assuming the feed composition is fixed at $\bar{c}_e$, the *preceding N-composition column model* is written by

$$\dot{c} = f_c(c, u), \quad c(0) = c_o, \quad y = h(c) := [\beta(c_{l_1}), \beta(c_{l_2})] \qquad (1)$$
$$c = (c_1, \ldots, c_N)', \quad u = (F, R, V)', \quad \dim(c, y, u) = (N, m, 3, 1)$$

In virtue of the afore stated modeling assumptions, the *actual column dynamics* are given by

$$\dot{c} = f_c(c, u) + \tilde{f}_c(c, \xi, d), \; c(t_o) = c_o, \; y = h(c) + \tilde{h}_c(c, \xi) + e_y \quad (2a)$$
$$\dot{\xi} = f_\xi(c, \xi, d, \dot{d}), \qquad \xi(t_o) = \xi_o, \; d = (u, e_u, d_e), \dim \xi = n_\xi \quad (2b)$$

with concentration (or unmodeled) state x (or ξ), actuator error e_u, and unmodeled exogenous input d_e. The unmodeled dynamics (2b) have slow and fast components due to the modeling-measurement errors, including holdup and enthalpy QSS assumptions. Thus, the N-composition model (1) is the actual system (2) with the modeling assumption $(\tilde{f}_c, \tilde{h}_c, e_y) = 0$.

2.2 *Adjustable*-structure estimation model

Following a previous binary distillation column GE (Alvarez and Fernandez, 2009) study with the estimation model regarded as design degree of freedom, rewrite the actual column dynamics (1) in terms of n ≤ N modeled compositions (x):

$$\dot{x} = f(x,u) + \tilde{f}(x, \chi, d, u), \; x(t_o) = x_o, \; y = h(x) + \tilde{h}(x, \chi) + e_y \quad (3a)$$
$$\dot{\chi} = f_\chi(x, \chi, d, \dot{d}), \; \chi(t_o) = \chi_o, \; (x, x_\varnothing) = I_c c, \; \chi = (x_\varnothing, \xi) \qquad (3b)$$

where $x_\varnothing$ are the unmodeled concentrations and χ is the augmented unmodeled state. The vector f depends only on the modeled concentrations x, due to a key modeling assumption made for estimator decentralization purposes (Alvarez and Fernandez, 2009): (i) f is the part of f_c that describes x, and is calculated with the unmodeled state at an average constant value ($\bar{x}_\varnothing$), as the related error can be effectively compensated by the GE integral action when the estimation structure is adequately chosen. In terms of κ_1 (or κ_2) *innovated sates* x_1 (or x_2) and (n - κ) *noninnovated states* (x_ι), the *actual dynamics* (2) are given by

$$\dot{x}_1 = f_1(x_1, u) + \tilde{f}_1(x, \chi, d, u), \; y_1 = h_1(x_1) + \tilde{h}_1(x, \chi) + e_1 \qquad (4a)$$
$$\dot{x}_2 = f_2(x_2, u) + \tilde{f}_2(x, \chi, d, u), \; y_2 = h_2(x_2) + \tilde{h}_2(x, \chi) + e_2 \qquad (4b)$$
$$\dot{x}_v = f_v(x_v, x_1, x_2, u) + \tilde{f}_v(x, \chi, d, u), \quad x_v(t_o) = x_{vo} \qquad (4c)$$
$$\dot{\chi} = \tilde{f}_\chi(x, \chi, d, \dot{d}), \; \chi(t_o) = \chi_o, \; x_1(t_o) = x_{1o}, \; x_2(t_o) = x_{2o} \qquad (4d)$$

where $(x_1, x_2, x_v, x_\varnothing) = I_c c, \qquad \dim(x_1, x_2, x_v) = (\kappa_1, \kappa_2, \kappa_v)$
$\kappa_1 + \kappa_2 = \kappa_\iota, \; \kappa_1 + \kappa_2 + \kappa_v = n \le N, \; (x_1, x_2) = x_\iota, \dim(x_\iota) = \kappa_\iota$

f_1 (or f_2) corresponds to x_1 (or x_2), and is calculated with some (average) constant value [$\bar{x}_1$(or $\bar{x}_2$), $\bar{x}_v$]. From the specialization of the general-purpose definition of model structure [Alvarez and Fernandez, 2009] to the binary column case, the definition of *column model structure* follows

$$\sigma = (\kappa, x_\iota - x_v), \; \kappa = (\kappa_1, \kappa_2), \; \kappa_1 + \kappa_2 = \kappa_\iota \le n, \; x_\iota = (x_1^\iota, x_2^\iota)' \quad (5)$$

where κ is the *estimation order* vector, x_ι-x_v is the innovated-noninnovated state partition, and x_1 (x_2) are κ_1 (or κ_2) adjacent concentrations associated with the measurement y_1 (or y_2). Thus, from the enforcement of the modeling assumption

$$(\tilde{f}_1, \tilde{f}_2, \tilde{f}_v) = 0, \qquad (\tilde{h}_1, \tilde{h}_2) = 0, \qquad (e_1, e_2) = 0 \qquad (6)$$

upon the actual subsystem (4a-c), the *estimation model*, with estimation structure σ (5), follows:

$$\dot{x}_1 = f_1(x_1, u), \qquad x_1(t_o) = x_{1o}, \qquad y_1 = h_1(x_1) \qquad (7a)$$
$$\dot{x}_2 = f_2(x_2, u), \qquad x_2(t_o) = x_{2o}, \qquad y_2 = h_2(x_2) \qquad (7b)$$
$$\dot{x}_v = f_v(x_v, x_1, x_2, u), \quad x_v(t_o) = x_{vo} \qquad (7c)$$

2.3 *Adjustable-structure geometric estimator (GE)*

In virtue of the σ-detectability property of the N-composition staged model (7), the (possibly truncated) model state (x) can be on-line robustly estimated by the *geometric estimator (GE) with structure* σ:

$$\dot{\hat{x}}_1 = f_1(\hat{x}_1, u) + O_1^{\iota\,-1}(\hat{x}_1, u)\{\pi_1\hat{\iota}_1 + k_1(\zeta_1, \omega_1)[y_1 - h_1(\hat{x}_1)]\},$$
$$\hat{x}_1(t_o) = \hat{x}_{1o}; \qquad \dot{\hat{\iota}}_1 = \omega_1^{\kappa_1+1}[y_1 - h_1(\hat{x}_1)]\}, \quad \hat{\iota}_1(0) = \hat{\iota}_{1o} \qquad (8a)$$
$$\dot{\hat{x}}_2 = f_2(\hat{x}_2, u) + O_2^{\iota\,-1}(\hat{x}_2, u)\{\pi_2\hat{\iota}_2 + k_2(\zeta_2, \omega_2)[y_2 - h_2(\hat{x}_2)]\},$$
$$\hat{x}_2(t_o) = \hat{x}_{2o}; \qquad \dot{\hat{\iota}}_2 = \omega_2^{\kappa_2+1}[y_2 - h_2(\hat{x}_2)], \quad \hat{\iota}_2(0) = \hat{\iota}_{2o} \qquad (8b)$$
$$\dot{x}_v = f_v(\hat{x}_\iota, \hat{x}_1, \hat{x}_2, u) \qquad \hat{x}_v(t_o) = \hat{x}_{vo} \qquad (8c)$$

where: $\qquad k_i(\zeta_i, \omega_i) = [a_1^i(\zeta_i)\omega_i, \ldots, a_{\kappa_i}^i(\zeta_i)\omega_i^{\kappa_i}]' \qquad (9c)$

$$O_i^\iota(x_i, u) = [\beta'(c_{l_i})]e_i[I, A_i(x_i, u), \ldots, A_i^{\kappa_i+1}(x_i, u)], \; i = 1, 2 \quad (9a)$$
$$A_i(x, u) = \partial_x f(x_i, u), \; \pi_i = (0, \ldots, 0, 1)', \; \dim \pi_i = \kappa_i \qquad (9b)$$
$$|\beta'(c_{l_1})| \ge \varepsilon_T, \quad |\beta'(c_{l_2})| \ge \varepsilon_T \qquad (10a\text{-}b)$$

ζ_i (or ω_i) is the damping factor (or characteristic frequency) of the prescribed linear, noninteractive, pole assignable (*LNPA*) output error dynamics

$$\tilde{y}_i^{(\kappa_i+1)} + a_1^i(\zeta_i)\,\omega_i\tilde{y}_i^{(\kappa_i)} + \ldots + a_1^i(\zeta_i)\,\omega_i\tilde{y}_i^{(1)} + \omega_i^{\kappa_i+1}\tilde{y}_i = 0, \; i = 1, 2 \quad (11)$$

with coefficient sets $\{a_1, \ldots, a_{\kappa_1}\}_i$ determined by pole placement (Lopez and Alvarez, 1999). The invertibility of O_1 and O_2 is ensured by the tridiagonal state dependency of f_c and the sensor location condition (10) which amounts placing each sensor at a tray with temperature gradient larger than a minimum value (say, two degrees). For any model structure σ (5) (Alvarez and Fernandez, 2009): (i) the afore stated nonlocal robustness convergence feature holds with respect to the N-composition model (1) with decentralization, truncation, and actuator-measurement errors, and (ii) the rather simple GE tuning scheme applies to any structure. Thus, the adjustable structure-algorithm GE methodological framework offers the means to fairly compare the behavior of different structures, in the sense that the behavior differences are due to the structures itself and not to the tuning.

2.4 Estimation structure design problem

In view of the preceding adjustable-structure column GE approach, *our present problem* consists in, given a specific estimation objective, determining the two-measurement structure, which yields the best estimator behavior in terms of reconstruction speed, robustness and dimensionality. Technically speaking, the problem amounts to choosing the (complete or truncated) estimation model (7) and its σ-detectability structure (5), or equivalently: (i) the location l_1 (or l_2) of the temperature measurement y_1 (or y_2), (ii) the corresponding innovated concentrations x_1 (or x_2), and (iii) the noninnovated state (x_v).

2.5 Structure search methodology

From the perspective of a general-purpose mixed-integer optimization approach, in our 12-stage distillation column example, the N-composition model offers 527, 345 structural possibilities with 4,095 observable (or passive) ones structures, and the number of possibilities grows even more when model truncation is considered. Leaving aside the implementation complexity and difficulties of an optimization-based search method, in the spirit of the constructive control (Sepulchre, 1997) and GE (Alvarez and Fernandez, 2009) approaches, here the structural search will performed by exploiting the column staged feature in the light of the easy to compute version (Alvarez and Fernandez, 2009) of the GE detectability measures (Lopez and Alvarez, 2004), in two steps: (i) first, detectability measures will be used to draw candidate structures for a given estimation objective, and (ii) then, conclusive structural results will be obtained in terms of GE functioning.

2.6 Experimental case example

The proposed methodology will be illustrated and tested with experimental case example employed before to illustrate and test the theoretically drawn features and capabilities of the general-purpose GE approach (Alvarez and Fernandez, 2009): a methanol-water mixture feed F = 40 ml/min, at 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 feed concentration step increase (c_e: 0.2 → 0.4) was introduced, yielding: (i) an overall composition response that settled (≈ 40 min) at an intermediate separation steady-state ($c_B \approx 0.01$, $c_D \approx 0.79$), and (ii) a distillate (or bottoms) composition settling time of ≈ 15 (or 40) min. Finally, at t = 40 min, a reflux step increase (R/D: 0.2 → 1.5) was introduced, yielding: (i) an overall response that settled (≈ 60 min.) at a high-separation steady-state ($c_B \approx 0.15$, $c_D \approx 0.98$), and (ii) a distillate (or bottoms) composition settling time of ≈ 20 (or 50) min. The experimental data can be seen in (Alvarez and Fernandez, 2007 and 2009).

3. STRUCTURAL ANALYSIS

In this section, the dependency of the GE detectability measures (Lopez and Alvarez, 2004; Alvarez and Fernandez, 2007) over sensor location and innovated state dimension are analyzed to draw candidate structures for complete profile and two-effluent estimation purposes.

3.1 Detectability measures

To account for the effect of the decentralization-truncation performed in the passage from the complete N-composition (1) to the truncated-decentralized n-composition estimation model (7) with structure σ (5), the detectability measures (12) for the next N-composition model (13) with innovated-noninnovated state partition will be employed (Alvarez and Fernandez, 2009):

$$s_\iota = 1/\text{msv}(O), \quad c_\iota = \text{cn}(O) \qquad (12a\text{-}b)$$
$$s_v = \text{msv}(F), \quad c_v = \text{cn}(F); \quad \lambda_v = ½\, \text{lev}(F + F') < 0 \quad (12c\text{-}d)$$
$$\dot{x}_\iota = f_\iota(x_\iota, x_v, u), \quad x(0) = x_{\iota o}, \; y = h(x_\iota), \; \dim(x_\iota) = N \qquad (13a)$$
$$\dot{x}_v = f_v(x_\iota, x_v, u), \quad x_v(t_o) = x_{vo}, \qquad \dim(x_v) = N\text{-}n \quad (13b)$$

where $O(x, u) = \text{bd}\,(E_1^{\iota}, E_2^{\iota})'(x, u)$, $\quad A_i(x_i, u) = \partial_{x_\iota} f_\iota(x, u)$
$F(x, u) = [\partial_{x_v} f_v + \partial_{x_\iota} f_v O^{-1} D](x, u)$, $\quad A_v(x, u) = \partial_{x_v} f_v(x, u)$
$E_i^{\iota}(x, u) = \beta'(c_{l_i}) e_i(I, A_i, \ldots, A_i^{\kappa i-1})(x, u)$, $\quad i = 1, 2$
$D'(x, u) = \beta'(c_{l_i}) e_i(I, A_v, \ldots, A_v^{\kappa i-1})(x, u)$, $\quad (x_1^{\iota}, x_2^{\iota})' = x_\iota$

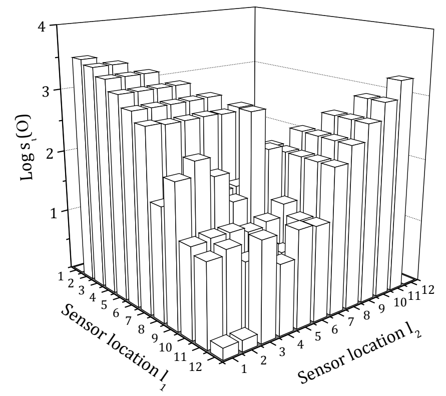
s_ι (or s_v) is the singularity measure equal to the inverse of the minimum singular value (msv) of the matrix O (or F), c_ι (or c_v) is the illconditioning measure equal to condition number (cn) of the matrix O (or F), and λ_v is the dominant frequency of the noninnovated dynamics, or equivalently, the negative of the smallest eigenvalue (lev) of the matrix (F + F')/2, O is the estimation matrix of the σ-structure model (13), and F is the Jacobian matrix of the noninnovated dynamics (13b). The illconditioning value c_ι (or c_v) measures the overshoot response of the innovated (or noninnovated) state estimation error to an initial estimate error, and the singularity value s_ι (or s_v) measures the asymptotic offset of the innovated (or noninnovated) state error due to persistent modeling errors, and the number λ_v measures the convergence rate of the noninnovated state error dynamics. In general, these measures can be taken over a column motion x(t) (Lopez and Alvarez, 2004). In our column case, the detectability measures will be computed at the intermidiate steady state (reached after ≈ 40 min).

3.2 Measurement locations

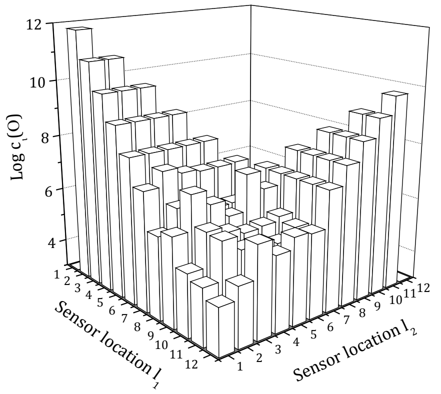
In Figure 1 are presented the singularity (s_ι) and ill conditioning (c_ι) measures (12) of the estimation matrix O (9a) as function of the sensor location pair (l_1, l_2), for a completely observable structure σ (5) with estimation order pair $\kappa = (\kappa_1, \kappa_2) = (6, 6)$ and $\kappa_\iota = \kappa_1 + \kappa_2 = 12 = n = N$ (i.e., complete model with observable structure), showing that: (i) the largest singularity and illconditioning values are obtained with the sensor stage location pair (l_1, l_2) ≈ (1 to 2, 12), (ii) the smallest singularity and illconditioning values are obtained with the sensor location $(l_1, l_2) \approx (1, 2)$ [or (11, 12)] with two adjacent sensors in the bottom (or top) of the column, followed by the sensor location $(l_1, l_2) \approx (5, 6)$ with two adjacent sensors above or below the feed tray (5). These consideration lead to the *following conclusions*: (i) the two sensors should not be in the same section, and (ii) the best location pair for complete profile estimation is given by

$$(l_1, l_2) = (2, 12) := (l_s, l_e) \quad (14)$$

meaning one sensor in stage $l_s = 2$ (tray one) [or $l_e = 12$ tray 10] of the stripping (or enriching section), precisely in the stage with the largest temperature and concentration stage-to-stage gradient.



a)



b)

Fig. 1: Dependency of the singularity s_ι and ill conditioning c_ι of the estimation matrix O on the sensor location pair (l_1, l_2), for comple observable structure σ (5) estimation order pair $\kappa = (\kappa_1, \kappa_2)$ and $\kappa_1 + \kappa_2 = 12$.

These location results are in agreement with location criteria employed in: (i) two-point temperature PI control of distillation columns (Tolliver, 1980; Castellanos-Sahagun et al., 2005), and (ii) previous distillation column studies with EKF (Baratti et al., 1995; Oisiovici and Cruz, 2000).

3.3 Innovated state dimension pair

Next, the sensor pair location (14) determined in the last section for the complete model (1), with observable structure κ (5), is kept fixed, and the dependency of the illconditioning c_ι (12a) and the speed parameter λ_v (12c) of the noninnovated dynamics upon the innovated state dimension (or equivalently, estimation order) pair $\kappa = (\kappa_s, \kappa_e)$ is examined, with κ_s (or κ_e) being the number of adjacent innovated states x_s (or x_e) associated with the measurement y_s (or y_e) of the stripping (or enriching) section. The resulting measure c_ι (or λ_v) is presented in Figure 2a (or 2b), showing that the illconditioning measure c_ι remains within a reasonable bound ($1 \le c_\iota \le 100$) for all the estimation order pairs with at most three innovated states per measurement [$(\kappa_s, \kappa_e) \le (3, 3)$]. As expected (Lopez and Alvarez, 2004): (i) the passive structure $(\kappa_s, \kappa_e) = (1, 1)$ yields the smallest possible value $c_\iota = 1$, and (ii) the speed parameter λ_v of the noninnovated dynamics is minimum ($\lambda_v = 0$) when the structure is observable with $(\kappa_s, \kappa_e) = (6, 6)$. These results are consistent with the general-purpose GE approach (Alvarez y Fernandez, 2009): (i) as the number of innovated states grows, the reconstruction speed grows and the robustness decreases, and (ii) the maximum robustness is obtained with the passive structure $(\kappa_s, \kappa_e) = (1, 1)$, and (iii) the maximum reconstruction speed is obtained with the observable structures $(\kappa_s, \kappa_e) = (6, 6)$.

3.4 Candidate structures

From the preceding structural analysis the next results follow. For *complete profile estimation*, the candidate models are decentralized versions of the N-concentration model (1) with structure σ (5):

$$\dot{c}_s = f_s(c_s, u), \qquad \dot{c}_e = f_e(c_e, u), \quad y = h(c) \quad (15a)$$
$$(\kappa_s, \kappa_e) \le (3, 3), \quad (l_s, l_e) = (2, 12) \quad (15b)$$

For *two-effluent estimation*, the candidate model is the truncated-decentralized model with passive structure σ (5):

$$\dot{c}_1 = \{(R + F)(c_2 - c_1) - V[\varepsilon(c_1) - c_1]\}/M_1, \quad (16a)$$
$$\dot{c}_2 = \{(R + F)(\bar{c}_3 - c_2) - V[\varepsilon(c_2) - \varepsilon(c_1)]\}/\eta^{-1}(R + F), \; y_s = \beta(c_2)$$
$$\dot{c}_{12} = \{R[\varepsilon(c_{12}) - c_{12}] - V[\varepsilon(c_{12}) - \varepsilon(\bar{c}_{11})]\}/\eta^{-1}(R), \quad y_e = \beta(c_{12})$$
$$(\kappa_s, \kappa_e) = (1, 1), \qquad (l_s, l_e) = (2, 12) \quad (16b)$$

4. STRUCTURAL RESULTS

Having as point of departure the suggestive structural results (15, 16) of the last section, in the present section conclusive results are obtained by assessing the candidate structures in terms of reconstruction speed and robustness.

4.1 Estimator tuning and convergence

The column (or holdup) dominant (or fastest) frequency ω_c (or ω_η) was determined from the experimental data and the detailed model (1), the estimator frequency ω is written as n_ω times ω_n, and the adjustable constants (20) are listed next:

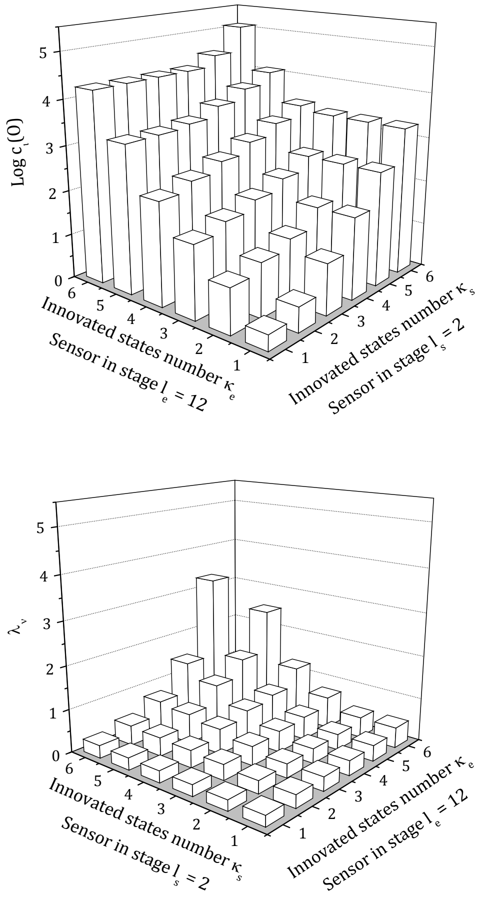
$$(\omega_c, \omega_\eta) \approx (1/15, 1)\ \text{min}^{-1}; \ \zeta_s, \zeta_e, \omega_s = \omega_e = \omega = n_\omega \omega_c \quad (17\text{-}18)$$

Thus: (i) there are three adjustable gains $(\zeta_s, \zeta_e, n_\omega)$, and (ii) the limit upper ω^+ is related to ω_η. From the specialization to the column case of Lemma and Proposition 1 in (Alvarez and Fernandez, 2009): (i) the GE error dynamics is robustly stable if the stabilizing term λ_s dominates the potentially destabilizing one λ_d (λ_s and λ_d defined in Alvarez and Fernandez, 2009), according to inequality (19), or equivalently, if: (i) the related threshold equation (20) has two strictly positive and sufficiently separated roots (ω^- and ω^+) for ω, and (ii) the gain frequency ω (18) of the prescribed LNPA output error dynamics (11) is chosen so that the low-high gain conditions (21) are met:

$$\lambda_s(\omega, \zeta, \sigma) - \lambda_d(\omega, \zeta, \sigma) := \lambda(\omega, \zeta, \sigma) > 0, \ \zeta = (\zeta_s, \zeta_e) \quad (19)$$

$$\lambda(\omega, \zeta, \sigma) = 0 \quad \Rightarrow \quad \exists \quad \omega = \omega^-(\zeta, \sigma), \quad \omega^+(\zeta, \sigma) \quad (20)$$

$$0 < \omega^-(\zeta, \sigma) < \omega < \omega^+(\zeta, \sigma) \quad (21)$$



a)

b)

Fig. 2: Dependency of the singularity (or noninnovated-dynamics speed parameter) s_ι (or c_ι) of the estimation matrix O (or Jacobian matrix F) on the dimension $\kappa = (\kappa_s, \kappa_e)$ of the innovated state pair x_s-x_e, for the sensor location $(l_s, l_e) = (2, 12)$

The meaning of these conditions and their dependency on κ_ι ($= \kappa_1, \kappa_2, \kappa_3$ with $\kappa_1 < \kappa_2 < \kappa_3$) are depicted in the Figure 1b of Alvarez and Fernandez (2009): (i) the fulfilment ($\kappa_\iota = \kappa_1$) or violation ($\kappa_\iota = \kappa_2, \kappa_3$) of the conditions, and (ii) as the estimation order κ_ι grows, the convergence gain (ω^+, ω^-) decreases, and eventually vanishes. In our column problem, we shall be interested in the interplay between structure, behavior, and tuning (ζ_s, ζ_e, ω, ω^-, ω^+, $\Delta\omega$).

4.2 Entire profile estimation

First, the GE estimator (8) was run with the candidate structures (κ_s, κ_e) = (1, 1), … (6, 6), finding that the best behavior was attained with (κ_s, κ_e) = (3, 3), followed by (2, 2). In Figure 3 are presented the results for (κ_s, κ_e) = (1, 1), (3, 3), and (6, 6), and the corresponding gain tuning limit results are listed in Table 1. The structure with three innovated states per measurement yields the best speed versus robustness behavior, with a reasonable gain interval (ω^+, ω^-). In agreement with the convergence-tuning theoretical derivations (Alvarez and Fernandez, 2009): (i) the passive (or observable) structure yields the slowest (or fastest) reconstruction rate with the largest (smallest) robustness, or equivalently, the largest (or smallest) gain interval $\Delta\omega$, and (iii) to avoid oscillatory response, the damping factor $\zeta_{s/e} = 2^{1/2}$ (or 1.5) is used for observable (or passive) innovation (Alvarez and Lopez, 1999).

4.3 Two-effluent estimation

In this case, the three-state model with two decoupled subsystems and passive innovation candidate structure (15) was implemented as well as several other neighbouring structures, finding that, the candidate structure yielded the best behavior with the least number of states, followed closely by some neighboring structures. The corresponding tuning and behavior are listed in Table 2 and Figure 4, respectively. As it can be seen in the Figure 4, for effluent estimation purposes, the truncated model outperforms the complete one, and this verifies the effectiveness of setting the model dimension as design degree of freedom. Comparing with the complete model-based estimation cases, the truncated model with single-stage innovation per measurement yields faster and more robust effluent estimates.

Table 1. Tuning for entire profile estimation.

y	κ	ζ	ω^-	ω	ω^+	$\Delta\omega$	n_ω
T_2, T_{12}	6, 6	$2^{1/2}$	1/15	2/5	8/15	7/15	6
T_2, T_{12}	3, 3	1	1/15	2/3	4/5	11/15	10
T_2, T_{12}	1, 1	3/2	1/15	4/5	14/15	13/15	12

Table 2. Tuning for two-effluent estimation.

n	κ	ζ	ω^-	ω	ω^+	$\Delta\omega$	n_ω
12	1, 1	3/2	1/15	4/5	14/15	13/15	12
3	1, 1	3/2	1/15	14/15	1	14/15	14

5. CONCLUSIONS

The problem of drawing the structure for best estimator behavior with respect to a specific concentration estimation task has been resolved for a binary distillation column with two temperature measurements and experimental data. It was found that: (i) the (12-concentration) profile must be estimated with the complete model, six innovated concentrations (three per measurement), and a 6-concentration open-loop observer module, and (ii) the two-effluent concentration must be estimated with a three-stage truncated model, two innovated concentrations, (one per measurement), and one noninnovated module. In the complete (or two-effluent) estimation case, the GE consists of 5 (or 14) ODE's, which are considerably less than the 72 ODEs required by an EKF implementation.

The proposed approach: (i) resolves the structure-algorithm estimation design problem in a way that is more effective and simpler than the ones of previous studies, and (ii) is a point of departure to address the multi-component case.

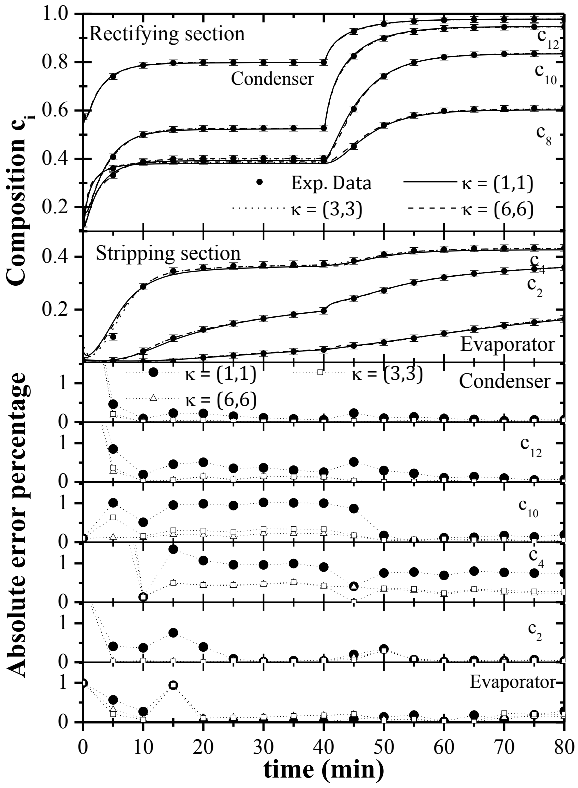


Fig. 3. Profile estimation with two sensors (l_s = 2, l_e = 12) and complete model.

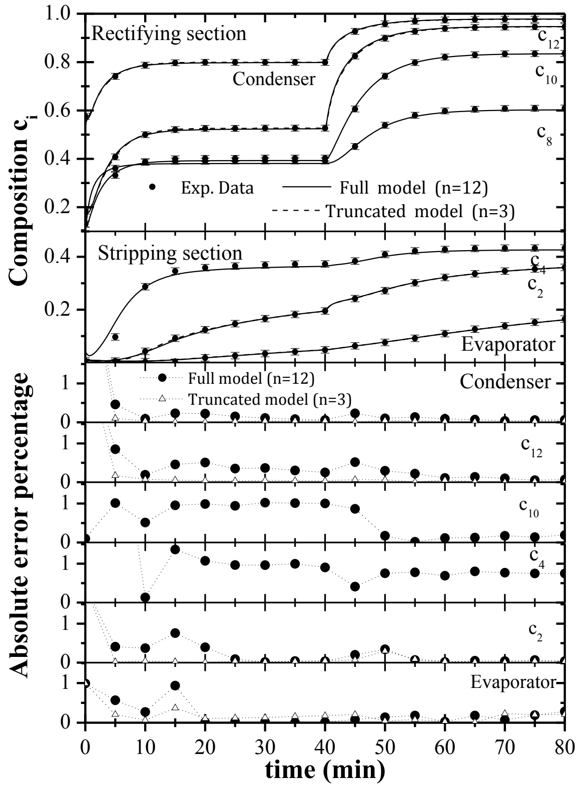


Fig. 4. Two-effluent estimation with two sensors (l_s = 2, l_e = 12) and truncated model.

REFERENCES

Alonso, A. A., Kevrekidis, I. G., Banga, J. R. and Frouzakis, C. E. (2004). Optimal sensor location and reduced order observer design for distributed process systems, *Comput. Chem. Eng.*, 28(1): 27-35

Alvarez, J. and Lopez, T. (1999). Robust Dynamic State Estimation of Nonlinear Plants, *AIChE J.*, 45(1): 107-123

Alvarez, J. (2000). Nonlinear state estimation with robust convergence, *J. Process Control*, 10(1): 59-71

Alvarez, J. and Fernandez, C. (2007). Constructive estimation design for binary distillation columns, *IFAC-DYCOPS 2007*, Preprints (II): 75-80

Alvarez, J. and Fernandez, C. (2009). Geometric estimation of nonlinear process systems, *J. Process Control*, 19(2): 247-260.

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

Bian, S. and Henson, M. A. (2006). Measurement selection for on-line estimation of nonlinear wave models for high purity distillation columns, *Chem. Eng. Sci.*, 61(10): 3210-3222

Castellanos-Sahagun, E., Alvarez-Ramírez, J. and Alvarez, J. (2005). Two-point temperature control structure and algorithm design for binary distillation columns, *Ind. Eng. Chem. Res.* 44: 142-152

Kadu, S. C., Bhushan, M. and Gudi, R. (2008). Optimal sensor network design for multirate systems, *J. Process Control*, 18: 594-609

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

Luyben, W. L. (1990). *Process modeling, simulation, and control for chemical engineers*. Nueva York, McGraw-Hill.

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

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

Singh, A. K. and Hahn, J. (2005). State estimation for high-dimensional chemical processes, *Comput. Chem. Eng.*, 29(11): 2326-2334

Tolliver, T. L. and McCune, L. C. (1980). Finding the Optimum Temperature Control Trays for Distillation Columns, *Instrum. Sci. Technol.* 27(9): 75-80

van den Berg, F. W. J., Hoefsloot, H. C. J., Boelens, H. F. M. and Smilde, A. K. (2000). Selection of optimal sensor position in a tubular reactor using robust degree of observability criteria, *Chem. Eng. Sci.*, 55: 827-837

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